Unit 7

Functions of several variables

Introduction

You are familiar with functions such as $f(x) = x^2$ and $g(t) = \sin^2 t$. You know how to differentiate and integrate such functions, and how to find their stationary points (including local maxima and minima). This is the usual stuff of calculus.

In describing the real world, however, we often meet functions of more than one variable. The volume of a brick depends on the lengths of its three sides. The rate of a chemical reaction depends on the concentrations of each of the reacting chemicals, and also on temperature. We may occasionally treat some of the variables as fixed parameters, but in general more than one variable is of interest, and we need to discuss functions of several variables. In this book you will see how we can extend the methods of calculus to functions of two and more variables.

The world that we inhabit has three spatial dimensions, and there are many physical quantities that vary throughout space. For example, the temperature may vary throughout a room. Since each point in the room can be represented by three coordinates (x, y, z), temperature is a function of the three variables x, y and z. We indicate this by writing the temperature function as $T(x, y, z)$.

In physics, quantities that depend on position throughout a whole region of space are called *fields*. There are many examples. We have just mentioned the temperature field; there are also electric fields, magnetic fields, gravitational fields, density fields, wind-velocity fields, and so on. The precise definitions of these fields need not concern us, but they all contain the essential idea of a physical quantity that varies with position.

Some physical quantities are vectors, having both magnitude and direction. For example, the velocity of a particle is a vector describing how fast the particle is moving *and in what direction*. In describing the wind-velocity field, we must specify a vector (the velocity of the wind) at each point in space. We therefore say that the wind-velocity field is a *vector field*. By contrast, the temperature field is a *scalar field* because temperature is a scalar quantity and has no direction associated with it.

This brief introduction has exposed two related ideas:

- We need to extend the methods of calculus to deal with functions of more than one variable.
- Nature provides many examples of functions of more than one variable in the form of fields that vary throughout regions of space. The fields that we will discuss are of two types: scalar fields and vector fields.

With this background, we can now outline the structure of this book.

Unit 7 introduces functions of more than one variable and shows how to differentiate them. This allows us to explore how sensitive these functions are to small changes in their variables, and to locate points at which the functions have maxima and minima.

Unit 8 describes how to integrate functions of more than one variable. For example, given an object of variable density, we will explain how its total mass can be found by integrating over the volume of the object. This is a so-called *volume integral*. We will also discuss integrals over surfaces, allowing us to find the surface areas of shapes such as spheres or cones.

Unit 9 looks at scalar and vector fields, and considers how to differentiate them. Such fields have special properties, and this leads to results beyond those introduced in Unit 7.

Unit 10 completes the book by discussing the integration of fields. Again, there are special results that apply to fields and take us beyond the integrals of Unit 8; these results turn out to be extremely powerful in physics and applied mathematics.

Because much of this book is largely concerned with fields, we will inevitably use physical examples – more so than elsewhere in this module. If you are unfamiliar with physics, be reassured. You need no prior understanding of physics, just a willingness to accept concepts such as temperature or velocity when they are used to illustrate mathematical ideas.

Study guide

This unit introduces functions of two or more variables. It explains how to differentiate these functions, and how to put the derivatives to use.

Section 1 introduces functions of more than one variable, and shows how they can be represented graphically in simple cases. It goes on to describe how these functions are differentiated with respect to individual variables.

Section 2 discusses the chain rule for functions of more than one variable. In fact, a number of different results go under this heading. These rules tell us how sensitive a function is to small changes in its variables, and how to find the derivative of a composite function – a function whose variables depend on other variables.

Section 3 briefly introduces Taylor polynomials for functions of more than one variable.

Finally, Section 4 investigates maxima, minima and other stationary points of functions of several variables. This is an important topic because many of the problems met in science, applied mathematics and economics reduce to finding the conditions under which functions have maximum or minimum values.

1 Partial differentiation

1.1 Notation for functions of one variable

Before describing functions of two and more variables, it is worth reviewing the notation used for functions of one variable. As an example, suppose that

$$z = f(x) = x^2 + 4. \tag{1}$$

Here x is called the *argument* of the function $f(x)$ or the *independent variable*, and z is called the *dependent variable*. If we insert a value for x in the expression $x^2 + 4$ on the right-hand side of equation (1), we get the corresponding function value. For $x = 3$, the function value is $f(3) = 3^2 + 4 = 13$. For $x = a$, the function value is $f(a) = a^2 + 4$.

As noted in Unit 1, similar notation is being used for different things. Equation (1) exhibits the *rule* that defines the function – in this case, 'take the square and add four' – so we may talk about the function $f(x)$. On the other hand, $f(3)$ and $f(a)$ represent particular *values* of the function. In spite of this clash, we will continue to use the $f(x)$ notation (and extend it to functions of more than one variable) – it is simply too useful to avoid.

Such 'abuse of notation' is practically unavoidable in subjects like physics, where mathematical symbols need to be related to physical concepts.

Moreover, in science, the symbols used to represent functions are often chosen in a special way. If we are interested in how a quantity M depends on position x, we may denote the function that describes this dependence by $M(x)$. Note that the symbol M is used for both the quantity and the function. We might also be interested in how M depends on time t, and denote the corresponding function by $M(t)$. This notation keeps us alert to the fact that both functions describe how the quantity M varies, but with respect to different variables. It avoids cluttering our descriptions with arbitrary new symbols whose physical meaning may be rapidly forgotten.

Suppose that the temperature T varies with position x along a rod. With T measured in degrees Celsius and x in metres, we might have

$$T = T(x) = 100e^{-x} \quad \text{for } 0 \le x \le 1.$$

The symbol T on the extreme left is the dependent variable, and x is the independent variable. The way in which T depends on x is described by the function $T(x) = 100e^{-x}$, which has x as its argument. The domain of this function is the region $0 \le x \le 1$.

1.2 Functions of more than one variable

The notation used for functions of a single variable is readily extended to functions of two or more variables. For example, the volume of the cone shown in Figure 1 is given by the formula $V = \frac{1}{3}\pi r^2 h$, where h is the height of the cone and r is the radius of its base. This can be described by a *function of two variables*:

$$V(h, r) = \tfrac{1}{3}\pi r^2 h.$$

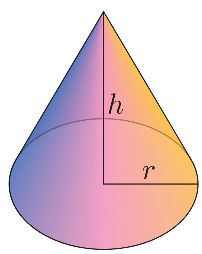


Figure 1 A cone of height h and base radius r

The arguments of this function are h and r. We can also say that h and r are the independent variables, and that the volume of the cone, V, is the dependent variable. For physical reasons, h and r are both positive numbers (measured in metres, say) so the domain of the function $V(h,r)$ is $0 < h < \infty$, $0 < r < \infty$.

The volume of the cone can be expressed in terms of other independent variables. The area of the base of the cone is $A = \pi r^2$, so the volume of the cone is $V = \frac{1}{3}Ah$, and this can be described by the function

$$V(h,A) = \tfrac{1}{3}Ah.$$

Note that the symbol V has been used for the physical quantity 'volume' and for two different functions, $V(h,r)$ and $V(h,A)$. Fortunately, the distinction between quantities and functions is generally clear from context, and the functions $V(h,r)$ and $V(h,A)$ are distinguished by the contents of their round brackets. Where there is a risk of ambiguity, guiding words will be supplied.

A second example is provided by temperature measured over a region. Suppose that we measure temperature on the surface of a horizontal disc of radius $R = 3$ (in metres). We describe points on the surface of the disc by Cartesian coordinates x and y (in metres), with the origin taken to be at the centre of the disc (Figure 2).

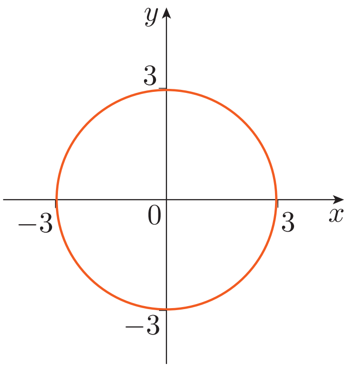


Figure 2 The Cartesian coordinate system used to specify points on a disc

The temperature may vary over the disc, but each point on the disc will have a well-defined temperature T, measured in degrees Celsius. We can represent the temperature variation over the entire surface of the disc by a function $T(x,y)$. For example, we might have

$$T(x,y) = 100\,e^{-(x^2+y^2)/10} \quad \text{on the disc.} \tag{2}$$

Here we use the symbol T for the temperature function on the disc, and it has arguments x and y. We can also say that x and y are the independent variables, and T is the dependent variable. The values of x and y are restricted because the formula in equation (2) applies only on the disc, and not elsewhere. The domain of the function is therefore the surface of the disc, i.e. the collection of points (x,y) with $x^2 + y^2 \le 9$.

Given the temperature function, it is a simple matter to calculate the temperature at any point on the disc. For example, at the point $(x,y) = (1,2)$, the temperature (in degrees Celsius) is

$$T(1,2) = 100\,e^{-(1^2+2^2)/10} = 100\,e^{-0.5} \simeq 60.7.$$

In this case, the point $(2,1)$ has the same temperature as the point $(1,2)$, but this is an accidental feature of the function that we have chosen. In general, the function value $f(a,b)$ is not the same as the function value $f(b,a)$, as you will see in the following exercise.

Exercise 1

Given $f(x,y) = 3x^2 - 2y^2$, evaluate the following.

(a) $f(2,3)$ (b) $f(3,-2)$ (c) $f(a,b)$ (d) $f(b,a)$

(e) $f(2a,b)$ (f) $f(a-b,0)$ (g) $f(x,2)$

1.3 Graphical representations

There are three main ways of visualising functions of two variables:

- Give a perspective view of a surface that represents the function.
- Show one or more slices through the surface.
- Draw a contour map.

All of these methods will be used in this unit, and we briefly introduce them now.

Perspective view of a surface

We can get a good overall understanding of a function $f(x,y)$ by plotting a 'three-dimensional graph'. The two independent variables x and y are plotted in the horizontal xy-plane, and the corresponding function values $z = f(x,y)$ are plotted along the vertical z-axis. Normally, the independent variables cover a continuous range and the function values vary smoothly, so we get a continuous surface, which can be viewed in perspective.

For example, Figure 3(a) is a three-dimensional graph of the function $f(x,y) = x^2 + y^2$. This shape is called a *circular paraboloid*, and is used in radio telescopes to focus a parallel beam to a single point (Figure 4(a)). Figure 3(b) is the graph of $f(x,y) = x^2 - y^2$. This shape is called a *hyperbolic paraboloid*, and has gained popularity with architects because it is eye-catching and relatively easy to construct (Figure 4(b)).

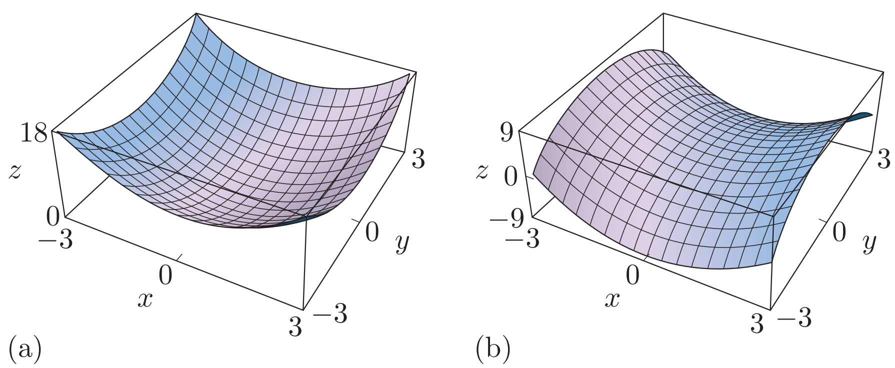


Figure 3 Three-dimensional graphs of (a) $f(x,y) = x^2 + y^2$ and (b) $f(x,y) = x^2 - y^2$

(a) (b)

Figure 4 (a) Radio telescopes have dishes that are circular paraboloids. (b) The roof of a station in Warsaw is shaped as a hyperbolic paraboloid.

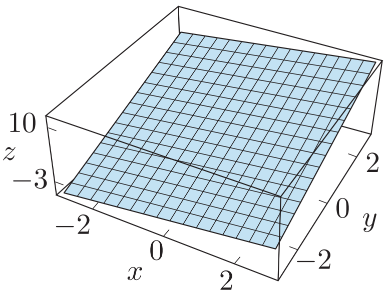


Figure 5 Part of the plane representing the function $f(x,y) = x + 2y + 3$

An important function of two variables is

$$f(x,y) = Ax + By + C, \tag{3}$$

where A, B and C are constants. This is a *linear function* of x and y, and when we plot it we get a plane. Conversely, the *equation of a plane* in three-dimensional space is given by equation (3). For example, the plane passing through the points $(-2,-2,-3)$, $(0,0,3)$ and $(2,2,9)$, and extending indefinitely, is given by the surface

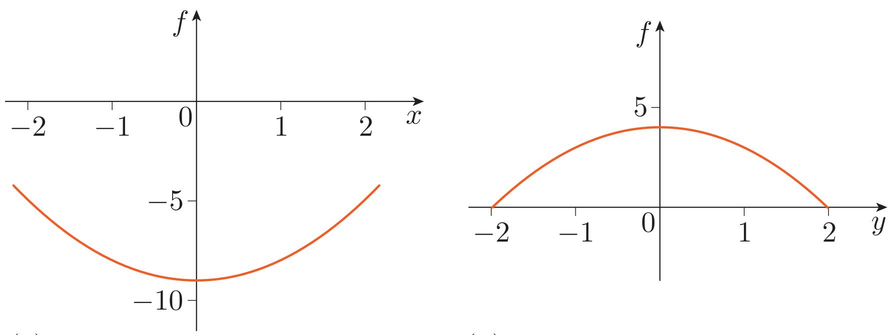
$$z = f(x,y) = x + 2y + 3.$$

A portion of this surface is shown in Figure 5.

Graphs of section functions

A second way of visualising a function of more than one variable is to fix the values of all but one of its variables, and then plot a graph showing its dependence on the remaining variable.

For example, given $f(x,y) = x^2 - y^2$, we can set $y = 3$ and then plot a graph of $f(x,3) = x^2 - 9$ against x, as in Figure 6(a). Or we can set $x = 2$ and plot a graph of $f(2,y) = 4 - y^2$ against y, as in Figure 6(b).



(a) (b)

Figure 6 Graphs of $f(x,y) = x^2 - y^2$ with one variable held constant: (a) graph of $f(x,3)$ against x; (b) graph of $f(2,y)$ against y

Figure 6(a) is obtained by taking a vertical section (or slice) through the three-dimensional graph in Figure 3(b). The slice is parallel to the x-axis

at the fixed value $y = 3$. Similarly, Figure 6(b) is obtained by taking a vertical slice parallel to the y-axis at the fixed value $x = 2$. Any function of the form $f(x, a)$ or $f(b, y)$, where a and b are constants, is called a **section function**. By itself, a single section function provides limited information: if y is held constant, the section function tells us only about the dependence on x at one fixed value of y, and it tells us nothing about the dependence on y. Nevertheless, a series of section functions taken at various fixed values of y, and various fixed values of x, can provide a great deal of useful information.

Contour maps

Finally, a function of two variables can be visualised using a *contour map*. You may be familiar with this idea from topographical maps (such as those produced by Ordnance Survey in the UK). Here the height of the land is described by a function $h(x, y)$, where x and y are position coordinates in a horizontal plane. The map shows a series of lines joining points of the same height; the example in Figure 7 shows heights between 5000 m below sea level and 3000 m above sea level.

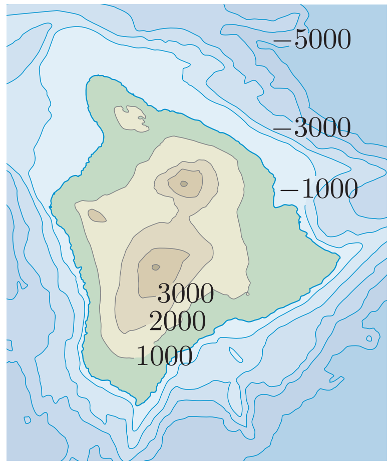


Figure 7 A contour map of Hawaii and the surrounding ocean floor

For any smooth function $f(x, y)$, we can plot a similar contour map. The x and y variables (whether they are position coordinates or not) are plotted in the plane of the page, and a curve is drawn in the xy-plane connecting neighbouring points where the function has a fixed value, say $f = c_1$. This is repeated for a series of values $c_1, c_2, c_3, \ldots$, giving a family of curves. A number is written beside each curve to indicate the value to which it refers. The curves are called **contour lines**, and the entire diagram is called a **contour map**.

Contour maps for the functions $f(x, y) = x^2 + y^2$ and $f(x, y) = x^2 - y^2$ are shown in Figures 8(a) and 8(b). To make sure that you are reading these contour maps correctly, you should compare them with Figures 3(a) and 3(b).

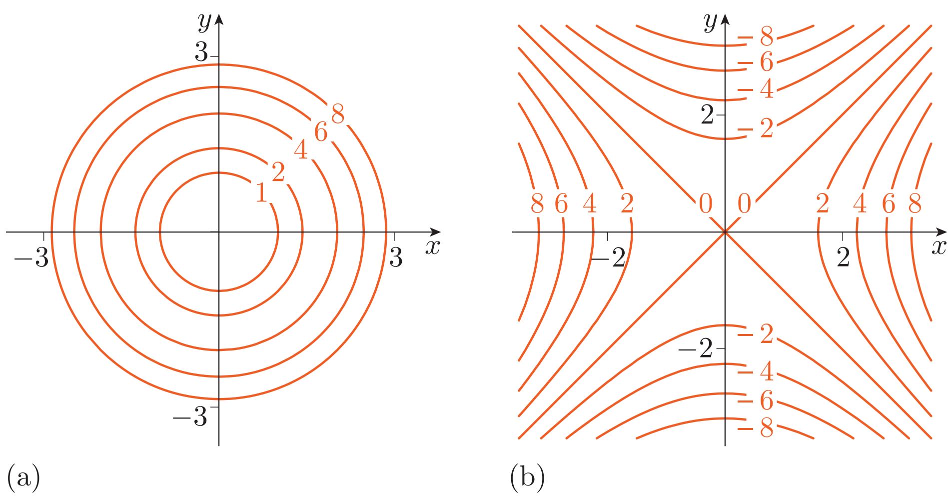


Figure 8 Contour maps for: (a) the function $f(x, y) = x^2 + y^2$; (b) the function $f(x, y) = x^2 - y^2$

Beyond two variables

Visualisation of functions of three or more variables is harder. We can always plot section functions, and for a function $f(x, y, z)$ we can plot the equivalent of a contour map, but in three dimensions. Here, neighbouring points with the same function value form a surface, known as a **contour surface**. For example, the function

$$f(x, y, z) = \frac{1}{\sqrt{x^2 + y^2 + z^2}}$$

has the fixed value $1/R$ at points where $x^2 + y^2 + z^2 = R^2$. These points lie on the surface of a sphere, so the contour surfaces of this function are concentric spheres centred on the origin. One of these could be shown in a perspective view, or we could show a cross-section through many of them. This is what has been done in Figure 9. Note that the concentric circles in this case are not contour lines, but are cross-sections through spherical contour surfaces, which extend equally above and below the horizontal plane of the page.

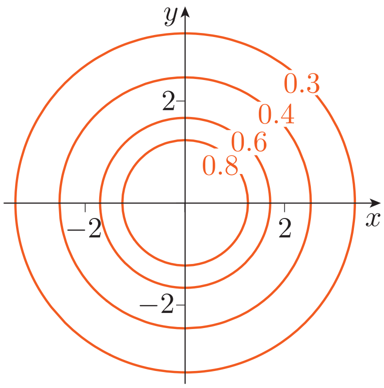


Figure 9 A cross-section in the $z = 0$ plane through the spherical contour surfaces of $f(x, y, z) = 1/\sqrt{x^2 + y^2 + z^2}$

Don't worry that you can't see things in more than three dimensions – no one can! This does not matter for our purposes. In order to motivate the key concepts for functions of many variables, the vital step is going from a function $f(x)$ of one variable to a function $f(x, y)$ of two variables. Once this step is made, we can easily extend our methods to functions of many variables without any need for diagrams.

1.4 First-order partial derivatives

Suppose that a variable f depends on x, and this dependence is described by the function $f(x)$. Then we can calculate the derivative df/dx, and this tells us the slope of a graph of $y = f(x)$. Equivalently, it tells us the rate of change of f with respect to x.

We would like to extend these ideas – initially to a function $f(x, y)$ of two variables. Corresponding to the slope of the graph $y = f(x)$, we have the slope of the surface $z = f(x, y)$. Here we run into a new feature: *the slope of a surface depends on our direction of travel.*

Figure 10 At any given point, the slope of a road depends on the direction that it takes over the terrain

Let us imagine that the function $f(x, y)$ represents the height of a hill, expressed in terms of the Cartesian coordinates x and y of points in a horizontal plane. Starting at some point on the hill, you might choose to go in a direction that goes directly up the hill, climbing steeply, or you might choose to go in a more oblique direction across the face of the hill, climbing less steeply. Roads in mountainous country often meander over the terrain, with many hairpin bends designed to keep the magnitude of the slope within safe limits (Figure 10). The slope encountered at any given point depends on the line chosen for the road.

More generally, for any surface $z = f(x, y)$, the slope of the surface depends on the direction in which we move. In the next section, we will

find a way of calculating the slope in any given direction, but first, we concentrate on two special directions: the x-direction and the y-direction. For each of these directions, we can define a slope by differentiating $f(x,y)$ in an appropriate way. This leads to the concept of a partial derivative, which we will now explain.

Consider the surface $z = f(x,y)$ obtained from the function

$$f(x,y) = x + y^3 + 2x^2y^2. \tag{4}$$

Suppose that we want to find the slope of this surface in the x-direction at the point $x = 2$, $y = 3$. Because we want the slope in the x-direction, the value of y is fixed at the value $y = 3$, and we can substitute this into equation (4) to obtain the function

$$f(x,3) = x + 27 + 18x^2.$$

This is the section function at constant y, with $y = 3$. It is a function only of x, and can be differentiated with respect to x to give

$$\frac{d}{dx}f(x,3) = 1 + 36x. \tag{5}$$

This derivative is the slope of the surface $z = f(x,y)$ in the x-direction for any value of x and for $y = 3$. Finally, substituting $x = 2$ in equation (5), we conclude that the slope in the x-direction at the point $x = 2$, $y = 3$ is equal to $1 + 36 \times 2 = 73$.

A similar calculation gives the slope in the y-direction at $x = 2$, $y = 3$. In this case we substitute $x = 2$ in equation (4) to obtain the section function

$$f(2,y) = 2 + y^3 + 8y^2.$$

This can be differentiated with respect to the remaining variable y to give

$$\frac{d}{dy}f(2,y) = 3y^2 + 16y.$$

Then, substituting in the value $y = 3$, the slope in the y-direction at the point $x = 2$, $y = 3$ is $3 \times 9 + 16 \times 3 = 75$. So the slopes in the x- and y-directions are not the same.

We could carry out similar calculations for any values of x and y in the domain of $f(x,y)$. At any given point, we can find the slope of $z = f(x,y)$ in the x-direction by differentiating with respect to x while treating y as a constant. Similarly, we can find the slope in the y-direction by differentiating with respect to y while treating x as a constant. Derivatives of this type, where certain variables are held constant, are known as *partial derivatives*, and they are written using curly dees as

$$\frac{\partial f}{\partial x} \quad \text{and} \quad \frac{\partial f}{\partial y}$$

or equivalently, as

$$\partial f/\partial x \quad \text{and} \quad \partial f/\partial y.$$

The expression $\partial f/\partial x$ is read as 'partial dee f by dee x'.

Partial derivatives

Given a function $f(x, y)$ of two variables x and y, the **partial derivative** $\partial f/\partial x$ is obtained by differentiating $f(x, y)$ with respect to x while treating y as a constant. Similarly, the partial derivative $\partial f/\partial y$ is obtained by differentiating $f(x, y)$ with respect to y while treating x as a constant.

Both $\partial f/\partial x$ and $\partial f/\partial y$ are also called **first-order partial derivatives** because they involve a *single* differentiation.

The partial derivative $\partial f/\partial x$ is equal to the slope in the x-direction of the surface $z = f(x, y)$. It tells us the rate of change of f with respect to x when we move in the direction of increasing x, keeping y fixed. The partial derivative $\partial f/\partial y$ is equal to the slope in the y-direction of the surface $z = f(x, y)$. It tells us the rate of change of f with respect to y when we move in the direction of increasing y, keeping x fixed.

A more formal definition of first-order partial derivatives is

$$\frac{\partial f}{\partial x} = \lim_{\delta x \to 0} \frac{f(x + \delta x, y) - f(x, y)}{\delta x}, \tag{6}$$

$$\frac{\partial f}{\partial y} = \lim_{\delta y \to 0} \frac{f(x, y + \delta y) - f(x, y)}{\delta y}. \tag{7}$$

It is worth noting that the two terms in the numerator on the right-hand side of equation (6) have the same value of y, which corresponds to treating y as a constant. By contrast, the two terms in the numerator on the right-hand side of equation (7) have the same value of x, and this corresponds to treating x as a constant.

As with ordinary differentiation, we tend to bypass these formal definitions and use the familiar rules of calculus to calculate partial derivatives. The only new feature is that some variables must be treated as constants during the differentiation.

Finding a partial derivative is no harder than finding an ordinary derivative. Just remember that all variables except the one involved in the differentiation must be treated as constants throughout the calculation.

Example 1

Find the partial derivatives $\partial f/\partial x$ and $\partial f/\partial y$ of the function $f(x, y) = x + y^3 + 2x^2y^2$ in equation (4).

Solution

To find $\partial f/\partial x$, we differentiate with respect to x, treating y as a constant:

$$\frac{\partial f}{\partial x} = 1 + 0 + 4xy^2 = 1 + 4xy^2.$$

The effect of holding y constant differs from term to term. In the term y^3, partial differentiation with respect to x gives zero because the derivative of any constant is zero. In the term $2x^2y^2$, the expression $2y^2$ is a constant coefficient for x^2, and this coefficient is unchanged by the differentiation.

To find $\partial f/\partial y$, we differentiate with respect to y, treating x as a constant:

$$\frac{\partial f}{\partial y} = 0 + 3y^2 + 4x^2y = 3y^2 + 4x^2y.$$

The partial derivatives that we have just calculated are functions of x and y because they refer to a general point (x, y) in the domain of the function f. To find the value of a partial derivative at a particular point, we substitute appropriate values of x and y. For the function in the above example, we see that at the point $x = 2$, $y = 3$, the values of the partial derivatives are

$$\left.\frac{\partial f}{\partial x}\right|_{x=2,\, y=3} = 1 + 4 \times 2 \times 9 = 73,$$
$$\left.\frac{\partial f}{\partial y}\right|_{x=2,\, y=3} = 3 \times 9 + 4 \times 4 \times 3 = 75.$$

These agree with the slopes calculated earlier using section functions. However, the use of partial derivatives is far more efficient because it gives the correct results for *all* values of x and y.

We have seen that the partial derivatives of $f(x, y)$ are functions of x and y. This is sometimes made explicit by using the alternative notations $f_x(x, y)$ and $f_y(x, y)$ instead of $\partial f/\partial x$ and $\partial f/\partial y$. In this case, the subscript x or y indicates the variable with respect to which the derivative is being taken. At a particular point, where $x = a$ and $y = b$, the values of the partial derivatives are denoted by $f_x(a, b)$ and $f_y(a, b)$, which is more compact than curly dee notation.

$f_x(x, y)$ and $f_y(x, y)$ may be abbreviated to f_x and f_y.

Of course, the two independent variables need not be denoted by x and y; any variable names will do, as the next example shows.

Example 2

Given $f(u, v) = u^2 + \sin(uv)$, calculate $f_u\left(\frac{\pi}{2}, 1\right)$ and $f_v\left(\frac{\pi}{2}, 1\right)$.

Solution

Differentiating $f(u, v)$ partially with respect to u gives

$$f_u(u, v) = 2u + v\cos(uv),$$

so

$$f_u\left(\tfrac{\pi}{2}, 1\right) = \pi + \cos\left(\tfrac{\pi}{2}\right) = \pi.$$

Differentiating $f(u,v)$ partially with respect to v gives

$$f_v(u,v) = 0 + u\cos(uv),$$

so

$$f_v\left(\tfrac{\pi}{2},1\right) = \tfrac{\pi}{2}\cos\left(\tfrac{\pi}{2}\right) = 0.$$

Exercise 2

Given $g(\theta,\phi) = \sin\theta + \cos\phi\tan\theta$, find $\dfrac{\partial g}{\partial\theta}$ and $\dfrac{\partial g}{\partial\phi}$.

Exercise 3

(a) Given $f(x,y) = (x^2+y^2)e^{3x}$, find $f_x(x,y)$ and $f_y(x,y)$.

(b) What is the slope of the surface $z = f(x,y)$ in the x-direction at the point $(0,1)$?

The concept of a partial derivative can easily be extended to functions of more than two variables. For a function $f(x,y,z)$ of three variables, $\partial f/\partial x$ no longer represents the slope of a surface, but it does represent the rate of change of f with respect to x when the other variables y and z have fixed values. The partial derivative $\partial f/\partial x$ is calculated by differentiating $f(x,y,z)$ with respect to x while keeping y *and* z fixed (and similarly for the other partial derivatives). More generally, we keep all but one of the variables fixed and differentiate with respect to the remaining variable.

Example 3

Given $V(x,y,z) = (x^2+y^2+z^2)^{-1/2}$, calculate $\partial V/\partial x$, $\partial V/\partial y$ and $\partial V/\partial z$.

Solution

This differentiation uses the 'function of a function' rule.

Partial differentiation with respect to x, with y and z constant, gives

$$\frac{\partial V}{\partial x} = -\tfrac{1}{2}(x^2+y^2+z^2)^{-3/2} \times 2x = -\frac{x}{(x^2+y^2+z^2)^{3/2}}.$$

Partial differentiation with respect to y, with x and z constant, gives

$$\frac{\partial V}{\partial y} = -\tfrac{1}{2}(x^2+y^2+z^2)^{-3/2} \times 2y = -\frac{y}{(x^2+y^2+z^2)^{3/2}},$$

and partial differentiation with respect to z, with x and y constant, gives

$$\frac{\partial V}{\partial z} = -\tfrac{1}{2}(x^2+y^2+z^2)^{-3/2} \times 2z = -\frac{z}{(x^2+y^2+z^2)^{3/2}}.$$

(Because the function $V(x,y,z)$ is symmetric in x, y and z, the answers for $\partial V/\partial y$ and $\partial V/\partial z$ can be obtained from the answer for $\partial V/\partial x$ by interchanging symbols. This is a useful check in this case.)

Exercise 4

(a) Given $f(x, y, z) = (1 + x)^2 + (1 + y)^3 + (1 + z)^4$, calculate the partial derivatives $\partial f/\partial x$, $\partial f/\partial y$ and $\partial f/\partial z$.

(b) Find all the first-order partial derivatives of the function

$$f(x, y, t) = x^2y^3t^4 + 4x^2t^2 - 2xy + y.$$

1.5 Higher-order partial derivatives

You have seen that the first-order partial derivatives of a function $f(x, y)$ are themselves functions of x and y. For example, the first-order partial derivatives of the function $f(x, y) = x + y^3 + 2x^2y^2$ are

$$\frac{\partial f}{\partial x} = 1 + 4xy^2 \quad \text{and} \quad \frac{\partial f}{\partial y} = 3y^2 + 4x^2y, \tag{8}$$

as you saw in Example 1. We can go on to differentiate $\partial f/\partial x$ partially with respect to x to obtain

$$\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial x}(1 + 4xy^2) = 4y^2.$$

Each of $\partial f/\partial x$ and $\partial f/\partial y$ can be partially differentiated with respect to either x or y, so equations (8) also give

$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial y}(1 + 4xy^2) = 8xy,$$
$$\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = \frac{\partial}{\partial x}(3y^2 + 4x^2y) = 8xy,$$
$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) = \frac{\partial}{\partial y}(3y^2 + 4x^2y) = 6y + 4x^2.$$

These four functions, obtained by partially differentiating $f(x, y) = x + y^3 + 2x^2y^2$ twice, are called **second-order partial derivatives**.

Second-order partial derivatives are written down using a natural extension of the notation for first-order partial derivatives. In curly-dee notation, we define

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right), \quad \frac{\partial^2 f}{\partial y\,\partial x} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right),$$
$$\frac{\partial^2 f}{\partial y^2} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right), \quad \frac{\partial^2 f}{\partial x\,\partial y} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right),$$

and in the alternative subscript notation,

$$f_{xx}(x, y) = \frac{\partial^2 f}{\partial x^2}, \quad f_{yx}(x, y) = \frac{\partial^2 f}{\partial y\,\partial x},$$
$$f_{yy}(x, y) = \frac{\partial^2 f}{\partial y^2}, \quad f_{xy}(x, y) = \frac{\partial^2 f}{\partial x\,\partial y}.$$

The value of the partial derivative $f_{xx}(x,y)$ at a particular point $x=a$, $y=b$ is then written as $f_{xx}(a,b)$, with similar notation for the other second-order partial derivatives.

If you can partially differentiate once, then you can partially differentiate again, so you should have no problem in calculating second-order partial derivatives. The following example illustrates the technique.

Example 4

Determine the second-order partial derivatives of the function

$$f(x,y)=e^x\cos y+x^2-y+1.$$

Solution

We have

$$\frac{\partial f}{\partial x}=e^x\cos y+2x,\quad \frac{\partial f}{\partial y}=-e^x\sin y-1,$$

so

$$\frac{\partial^2 f}{\partial x^2}=\frac{\partial}{\partial x}(e^x\cos y+2x)=e^x\cos y+2,$$

$$\frac{\partial^2 f}{\partial y\,\partial x}=\frac{\partial}{\partial y}(e^x\cos y+2x)=-e^x\sin y,$$

$$\frac{\partial^2 f}{\partial y^2}=\frac{\partial}{\partial y}(-e^x\sin y-1)=-e^x\cos y,$$

$$\frac{\partial^2 f}{\partial x\,\partial y}=\frac{\partial}{\partial x}(-e^x\sin y-1)=-e^x\sin y.$$

Exercise 5

Given $f(x,y)=x\sin y$, calculate the second-order partial derivatives f_{xx}, f_{yx}, f_{yy} and f_{xy}, and evaluate them at $(2,\pi)$.

The second-order partial derivatives of a function $f(x,y)$ can be interpreted geometrically. Just as first-order partial derivatives tell us about the slopes of the surface $z=f(x,y)$ in the x- and y-directions, so second-order partial derivatives tell us about the *rates of change* of these slopes when we move in various directions. In a derivative like f_{xx}, we differentiate twice with respect to x, holding y constant. The first differentiation gives us the slope of the surface in the x-direction. In general, this slope varies from point to point, and f_{xx} tells us how rapidly the slope in the x-direction changes as we move in the x-direction. Similarly, f_{yx} tells us how rapidly the slope in the x-direction changes as we move in the y-direction, and so on. Figure 11 illustrates these facts.

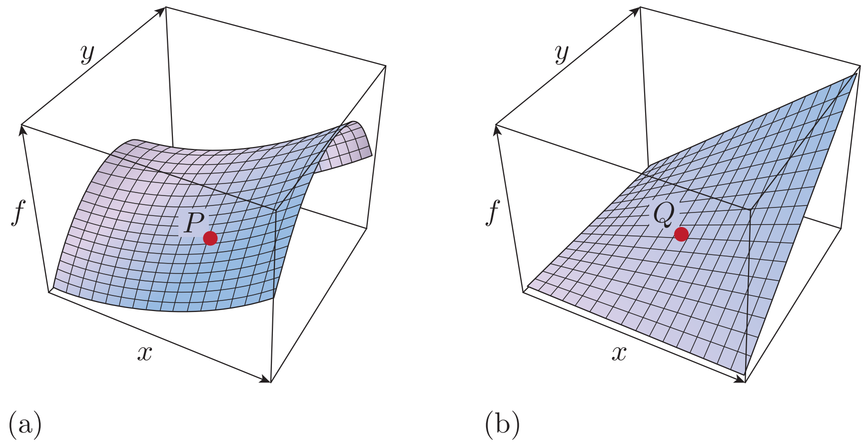


Figure 11 (a) At point P, $f_x > 0$ and $f_y > 0$, while $f_{xx} > 0$ and $f_{yy} < 0$. (b) At point Q, $f_x > 0$ and $f_y > 0$, while $f_{xy} > 0$ and $f_{yx} > 0$. Mixed partial derivatives such as f_{xy} and f_{yx} are non-zero for surfaces with a 'twist' in them.

Partial derivatives such as f_{xy} and f_{yx}, which involve differentiations with respect to different variables, are called **mixed partial derivatives**. In Example 4 and Exercise 5 (as well as in the work on the function at the beginning of this subsection) you can see that $f_{xy} = f_{yx}$. In fact, this property is guaranteed by the following theorem, which we do not prove.

Mixed partial derivative theorem

For any function $f(x, y)$ that is sufficiently smooth,

$$\frac{\partial^2 f}{\partial x\,\partial y} = \frac{\partial^2 f}{\partial y\,\partial x}, \quad \text{or equivalently,} \quad f_{xy} = f_{yx}.$$

A similar result applies to a smooth function $f(x_1, x_2, \ldots, x_n)$ of n variables. Again, the order of differentiation does not matter, so

$$\frac{\partial^2 f}{\partial x_i\,\partial x_j} = \frac{\partial^2 f}{\partial x_j\,\partial x_i} \quad \text{for all } x_i \text{ and } x_j.$$

When $x_i = x_j$ this is a trivial identity. The interest lies in the case $x_i \neq x_j$.

You do not need to know precisely what is meant by 'smooth' in this context. In fact, we will assume that the mixed partial derivative theorem applies to all the functions that you will meet in this module.

Exercise 6

Given $f(x, y) = e^{2x+3y}$, calculate $f_{xy}(0, 0)$ and $f_{yx}(0, 0)$.

Exercise 7

Given $f(x, t) = \cos(3x - 2t)$, find expressions for f_{xx} and f_{tt}. Hence write down a relationship between f_{xx} and f_{tt} that applies for all values of x and t for the given function.

2 Chain rules and the gradient vector

This section describes a number of rules known as *chain rules*. One of these rules will allow us to find the slope of a surface when we move in an arbitrary direction (not just parallel to the x- or y-axis). In the process, we will use partial derivatives to define a quantity called the *gradient vector*. This will be important later in this unit, and for later units in this book.

2.1 The chain rule for small changes

Suppose that a variable f depends on a single variable x, and this dependence is described by the function $f(x)$. Then we can write

Note how the notation is used: df/dx is a derivative, but $\delta f/\delta x$ is a quotient of two small quantities, δf and δx.

$$\frac{df}{dx} \simeq \frac{\delta f}{\delta x}, \tag{9}$$

provided that δx and the corresponding δf are small enough. Rearranging this equation gives an approximate formula for the change in f that accompanies a very small change in x:

$$\delta f \simeq \frac{df}{dx}\,\delta x. \tag{10}$$

We therefore see that df/dx determines the *sensitivity* of f to small changes in x. This is important when x is found by measurement and the function value $f(x)$ is deduced from it: if the derivative df/dx has a large magnitude for the value of x of interest, then we need to be very accurate in our measurement of x in order to make a reasonable estimate of f.

The key result is given in equations (18) and (19) below.

We would now like to extend this idea to a function $f(x, y)$ of two variables. In this case, we are interested in the change in f that arises when x and y *both* change by small amounts.

Figure 12 shows a contour map of a function $f(x, y)$.

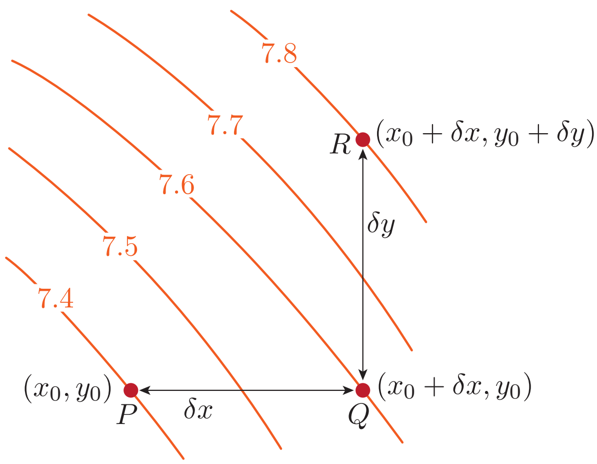


Figure 12 A contour map of a function $f(x, y)$. We consider the change in the value of f as we move from $P = (x_0, y_0)$ to a neighbouring point $R = (x_0 + \delta x, y_0 + \delta y)$.

We consider a point P in the xy-plane with coordinates (x_0, y_0), and a neighbouring point R with coordinates $(x_0 + \delta x, y_0 + \delta y)$. The change in f between these two points is

$$\delta f = f(x_0 + \delta x, y_0 + \delta y) - f(x_0, y_0). \tag{11}$$

The journey from P to R can be taken in two steps. In the first step, the value of y is held constant as we move from P to an intermediate point Q with coordinates $(x_0 + \delta x, y_0)$. In the second step, the value of x is held constant as we move from Q to R.

The change in the value of f in going from P to Q is

$$\delta f_1 = f(x_0 + \delta x, y_0) - f(x_0, y_0), \tag{12}$$

while the change in f in going from Q to R is

$$\delta f_2 = f(x_0 + \delta x, y_0 + \delta y) - f(x_0 + \delta x, y_0). \tag{13}$$

Adding equations (12) and (13), and comparing with equation (11), we see that

$$\delta f = \delta f_1 + \delta f_2. \tag{14}$$

You can check this for the case drawn in Figure 12: in this case, $\delta f = 7.8 - 7.4 = 0.4$, $\delta f_1 = 7.6 - 7.4 = 0.2$ and $\delta f_2 = 7.8 - 7.6 = 0.2$.

More generally, we can say that the change in f is *cumulative*. It is the sum of the change δf_1 obtained when moving in the x-direction and the change δf_2 obtained when moving in the y-direction. Fortunately, we can estimate δf_1 and δf_2 quite easily.

The journey from P to Q starts at the point (x_0, y_0) and makes a displacement δx with y held constant. The resulting change in f is $\delta f = \delta f_1$. By analogy with equation (9), we can therefore write

$$\frac{\partial f}{\partial x} \simeq \frac{\delta f_1}{\delta x}.$$

A partial derivative appears on the left because the journey is made *with y held constant*. This partial derivative is evaluated at point P, and so can be written as $f_x(x_0, y_0)$. Rearranging the equation, we therefore conclude that

$$\delta f_1 \simeq f_x(x_0, y_0)\,\delta x. \tag{15}$$

which is very like equation (10).

A similar argument can be given for the journey from Q to R. In this case, we start from the point Q, with coordinates $(x_0 + \delta x, y)$, and make a displacement δy with x held constant. In this case, we get

$$\delta f_2 \simeq f_y(x_0 + \delta x, y_0)\,\delta y. \tag{16}$$

In fact, this expression is needlessly complicated. If the function f_y varies smoothly, and δx is very small, then we can replace $f_y(x_0 + \delta x, y_0)$ by $f_y(x_0, y_0)$. You might think that this would introduce a small error, but this really does not matter. It turns out that the difference between $f_y(x_0 + \delta x, y_0)$ and $f_y(x_0, y_0)$ is proportional to δx, and because the last term in equation (16) includes a factor δy, the overall error introduced by

the replacement is proportional to $\delta x\,\delta y$. Such an error can be neglected in comparison to the terms that we are keeping. It is good enough to say that

$$\delta f_2 \simeq f_y(x_0, y_0)\,\delta y. \tag{17}$$

Finally, using equation (14), we see that the total change in f in going from a point (x_0, y_0) to a neighbouring point $(x_0 + \delta x, y_0 + \delta y)$ is

$$\delta f \simeq f_x(x_0, y_0)\,\delta x + f_y(x_0, y_0)\,\delta y.$$

This equation is valid throughout the domain of the function, so we can replace (x_0, y_0) by (x, y) to obtain our final result, the **chain rule**.

Chain rule for small changes

If $f(x, y)$ is a smooth function, then the change in the dependent variable f that occurs in response to small changes in x and y is

$$\delta f \simeq f_x(x, y)\,\delta x + f_y(x, y)\,\delta y. \tag{18}$$

Using curly dee notation, this rule can also be written in the form

$$\delta f \simeq \frac{\partial f}{\partial x}\,\delta x + \frac{\partial f}{\partial y}\,\delta y. \tag{19}$$

Example 5

The power P output by a star is given by the formula $P = kAT^4$, where A is the star's surface area, T is its surface temperature, and k is a constant. Derive a formula relating the fractional change in power output $\delta P/P$ to the corresponding fractional changes $\delta A/A$ and $\delta T/T$. You may assume that δA and δT are small enough for the chain rule to apply.

Solution

The first-order partial derivatives are

$$\frac{\partial P}{\partial A} = kT^4 \quad \text{and} \quad \frac{\partial P}{\partial T} = 4kAT^3,$$

so the chain rule gives

$$\begin{aligned}\delta P &= \frac{\partial P}{\partial A}\,\delta A + \frac{\partial P}{\partial T}\,\delta T \\ &= kT^4\,\delta A + 4kAT^3\,\delta T.\end{aligned}$$

Dividing both sides by $P = kAT^4$, we get

$$\frac{\delta P}{P} \simeq \frac{\delta A}{A} + 4\frac{\delta T}{T}.$$

The coefficient 4 multiplying $\delta T/T$ shows that a 1% increase in temperature produces an approximately 4% increase in power output.

Exercise 8

A quantity f is given by the function

$$f = f(x,y) = \frac{xy}{x+y}.$$

Find $\partial f/\partial x$ and $\partial f/\partial y$, and use the chain rule to estimate the small change in f that occurs when x changes from 1.00 to 1.01, and y changes from 4.00 to 3.99.

Note that $1/f = 1/x + 1/y$. Relationships like this occur when describing electrical circuits and optical lenses.

2.2 Other versions of the chain rule

In ordinary calculus, we often have to differentiate 'a function of a function'. Such a situation arises if the velocity $v = v(x)$ of a particle is given as a function of its position $x = x(t)$, which in turn is a function of time t. We can then write

$$v = v(x) = v(x(t)).$$

You know how to differentiate v with respect to t in such a case. We use the ordinary chain rule of calculus:

$$\frac{dv}{dt} = \frac{dv}{dx} \times \frac{dx}{dt}. \tag{20}$$

So if $v(x) = x^2$ and $x(t) = \sin t$, we have

$$\frac{dv}{dt} = \frac{dv}{dx} \times \frac{dx}{dt} = 2x \times \cos t = 2\sin t\cos t,$$

where we have used $x = \sin t$ in the last step. We could, of course, get the same result by noting that $v = x^2 = \sin^2 t$, and then differentiating $\sin^2 t$ directly; this makes *implicit* use of the chain rule, but we have chosen to be more explicit.

In this subsection, we will look at various generalisations of equation (20) to functions of more than one variable. All these results will be based on equations (18) and (19), and they are all called *chain rules.*

Differentiation with respect to a parameter

Suppose that x and y are both functions of the same variable t. For example, we could have

$$x = R\cos t \quad \text{and} \quad y = R\sin t, \tag{21}$$

where R is a constant and $0 \le t < 2\pi$. The variable t is called a **parameter**. It may represent time, but this is not essential; t could be any quantity that increases as we trace out a given path.

The fact that x and y are both functions of t implies that they are related to one another. In the present case, x and y both lie on a circle of radius R centred on the origin, as indicated in Figure 13, and we say that equations (21) provide a **parametric representation** of this circle. For a given value of t, they specify a definite point on this circle, and as t increases from 0 to 2π, we go once around the circle anticlockwise.

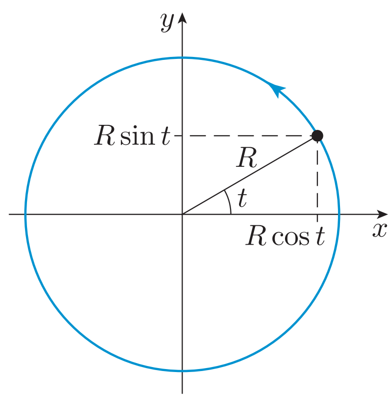


Figure 13 The parametric representation $x = R\cos t$, $y = R\sin t$, $0 \le t < 2\pi$, for points on a circle traced anticlockwise

Suppose that we are given a function $f(x, y)$ with x and y related to the parameter t by equations of the form $x = x(t)$, $y = y(t)$, so that

$$f = f(x(t), y(t)).$$

Then we can ask: what is the rate of change of f with respect to t? The answer is easily found by dividing both sides of equation (19) (the chain rule for small changes) by a small change δt:

$$\frac{\delta f}{\delta t} = \frac{\partial f}{\partial x}\frac{\delta x}{\delta t} + \frac{\partial f}{\partial y}\frac{\delta y}{\delta t}, \qquad (22)$$

and then taking the limit as δt tends to zero. This gives the following version of the chain rule.

Chain rule for differentiation with respect to a parameter

If $f = f(x(t), y(t))$, then

$$\frac{df}{dt} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt}. \qquad (23)$$

It is worth reflecting on the notation used here. Because $x(t)$ and $y(t)$ are functions of a single variable, we use the ordinary derivatives dx/dt and dy/dt, written with straight dees. By contrast, $f(x, y)$ is a function of two variables, so we use the partial derivatives $\partial f/\partial x$ and $\partial f/\partial y$, written with curly dees. Neither of these should be confused with ratios of small quantities, such as $\delta x/\delta t$ or $\delta y/\delta t$, which appear in equation (22).

Equation (23) is a direct extension of equation (20) to functions of two variables. We could, of course, substitute the functions $x(t)$ and $y(t)$ directly into $f(x, y)$ and carry out an ordinary differentiation with respect to t. Nevertheless, we will use equation (23) in the following example and exercises because this version of the chain rule is a valuable result with many uses and it is important to become familiar with it.

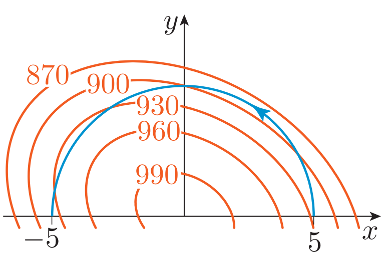


Figure 14 Contour map of a rock pinnacle (orange) with the projection on the xy-plane of the path followed by a mountaineer (blue)

Example 6

With distances measured in metres, the height h of a rock pinnacle depends on horizontal coordinates x and y according to the function

$$h(x, y) = 1000 - 3x^2 - 2xy - 4y^2$$
for $-10 < x < 10$ and $-10 < y < 10$.

A mountaineer follows the blue path shown in Figure 14, with her x- and y-coordinates given by the functions

$$x(t) = 5\cos(2t) \quad \text{and} \quad y(t) = 5\sin(2t) \quad \text{for } 0 \le t < \pi/2.$$

Use the chain rule to calculate dh/dt as a function of t.

Solution

The chain rule (in the form of equation (23)) tells us that

$$\frac{dh}{dt} = \frac{\partial h}{\partial x}\frac{dx}{dt} + \frac{\partial h}{\partial y}\frac{dy}{dt}.$$

The required partial derivatives are

$$\frac{\partial h}{\partial x} = -6x - 2y, \quad \frac{\partial h}{\partial y} = -2x - 8y,$$

while the derivatives of $x(t)$ and $y(t)$ are

$$\frac{dx}{dt} = -10\sin(2t), \quad \frac{dy}{dt} = 10\cos(2t).$$

We therefore obtain

$$\begin{aligned}\frac{dh}{dt} &= (-6x - 2y)(-10\sin(2t)) + (-2x - 8y)(10\cos(2t)) \\ &= 20\big((3x + y)\sin(2t) - (x + 4y)\cos(2t)\big).\end{aligned}$$

Finally, we use the parametric equations for x and y to express everything in terms of t. Direct substitution gives

$$\begin{aligned}\frac{dh}{dt} &= 100\big(3\cos(2t)\sin(2t) + \sin^2(2t) - \cos^2(2t) - 4\sin(2t)\cos(2t)\big) \\ &= 100\big(\sin^2(2t) - \cos^2(2t) - \sin(2t)\cos(2t)\big).\end{aligned}$$

Although it is not essential to do so, we could simplify this answer using trigonometric identities to obtain

$$\frac{dh}{dt} = -50\big(2\cos(4t) + \sin(4t)\big).$$

The final answer is the rate of change of h with respect to the parameter t. The significance of this parameter is left open in this question: it could represent time, in which case dh/dt would be the rate of change of height with respect to time, but this is not essential – in general, t could be any variable that increases along the path.

Exercise 9

Given $z = \sin x - 3\cos y$, use the chain rule to find the rate of change of z with respect to t, where x and y are given by the parametric equations $x = t^2$ and $y = 2t$.

Exercise 10

Given $z = y\sin x$, use the chain rule to find the rate of change of z with respect to t along the curve $(x(t), y(t))$, where $x = e^t$ and $y = t^2$. Evaluate this rate of change at $t = 0$.

The chain rule for a change of variables

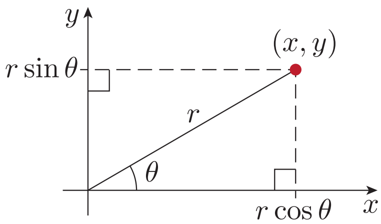


Figure 15 Polar coordinates: a point is defined by the distance r and the angle θ

At the start of this unit we used the example of temperature measured on the surface of a circular disc. This was described by a function $T(x, y)$ of the Cartesian coordinates x and y of points on the disc. But there is no compelling reason to choose Cartesian coordinates. We could equally well use *polar coordinates* r and θ, which are defined in Figure 15. From Figure 15, you can see that x and y are related to r and θ by the equations

$$x = r\cos\theta \quad \text{and} \quad y = r\sin\theta.$$

These equations imply that x and y are functions of r and θ, and we can express this by writing

$$x = x(r, \theta) \quad \text{and} \quad y = y(r, \theta).$$

The temperature function can then be regarded as a function of r and θ:

$$T(r, \theta) = T(x(r, \theta), y(r, \theta)).$$

This is an example of our deliberate 'abuse of notation'. $T(x, y)$ and $T(r, \theta)$ are different mathematical functions representing the same quantity, namely temperature.

We can ask: what is the rate of change of T with respect to r when θ is held constant? This is given by the partial derivative $\partial T/\partial r$, and we will now explain how to calculate this partial derivative from expressions for $T(x, y)$, $x(r, \theta)$ and $y(r, \theta)$ using another form of the chain rule.

Instead of using the r and θ of polar coordinates, let us consider a more general situation. Suppose that we are given a function $f(x, y)$ where the variables x and y are expressed in terms of two other variables, u and v, so that $x = x(u, v)$ and $y = y(u, v)$. Then we can write

$$f = f(x(u, v), y(u, v)),$$

and regard f as a function of u and v.

If x and y change by small amounts, we know that

$$\delta f = \frac{\partial f}{\partial x}\,\delta x + \frac{\partial f}{\partial y}\,\delta y.$$

Now divide both sides of this equation by δu, *under conditions in which v is held constant*. This division gives

$$\frac{\delta f}{\delta u} = \frac{\partial f}{\partial x}\frac{\delta x}{\delta u} + \frac{\partial f}{\partial y}\frac{\delta y}{\delta u},$$

and if we now take the limit as δu tends to zero *while holding v constant*, then the ratios of small quantities become *partial* derivatives. This leads to another form of the chain rule, used when we change variables from (x, y) to (u, v).

Chain rule for a change of variables

If $f = f(x, y)$ with $x = x(u, v)$ and $y = y(u, v)$, then

$$\frac{\partial f}{\partial u} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial u} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial u}. \tag{24}$$

By a similar argument, but dividing by δv while holding u constant,

$$\frac{\partial f}{\partial v} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial v} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial v}. \tag{25}$$

In these equations, $f(x, y)$ is a function of x and y, and $\partial f/\partial x$ implies that y is held constant, while $x(u, v)$ is a function of u and v, and $\partial f/\partial u$ implies that v is held constant, and so on. The best way to see how this works is with an example.

Example 7

Suppose that $f(x, y) = xy^2$, where $x = uv$ and $y = u^2 - v^2$. Use the chain rule to find $\partial f/\partial u$ in terms of u and v.

Solution

We have

$$\frac{\partial f}{\partial x} = y^2 \quad \text{and} \quad \frac{\partial f}{\partial y} = 2xy.$$

Also,

$$\frac{\partial x}{\partial u} = v \quad \text{and} \quad \frac{\partial y}{\partial u} = 2u.$$

So the chain rule (equation (24)) gives

$$\frac{\partial f}{\partial u} = vy^2 + 4uxy = v(u^2 - v^2)^2 + 4u^2v(u^2 - v^2),$$

which can (optionally) be tidied up to give

$$\frac{\partial f}{\partial u} = v(u^2 - v^2)(5u^2 - v^2).$$

Exercise 11

Suppose that $f(x, y) = x^2 + y^2$, where $x = 2u + 3v$ and $y = 3u - 2v$. Use the chain rule to find the partial derivatives $\partial f/\partial u$ and $\partial f/\partial v$, and evaluate your answers at $(u, v) = (1, 2)$.

Exercise 12

Suppose that $f(x, y) = x^2 - y^2$, where $x = r\cos\theta$ and $y = r\sin\theta$. Use the chain rule to find the partial derivatives $\partial f/\partial r$ and $\partial f/\partial \theta$.

2.3 Slope in an arbitrary direction

You saw earlier that the slope of a surface $z = f(x, y)$ depends on the direction of travel. The slope in the x-direction is given by the partial derivative $\partial f/\partial x$, and the slope in the y-direction is given by $\partial f/\partial y$, but what about the slope in an arbitrary direction?

We can answer this question using the chain rule, but first we must say what happens to the x- and y-coordinates when we move away from a given point (x_0, y_0) in a given direction.

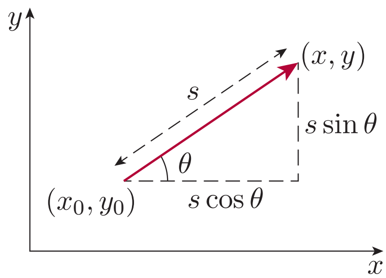


Figure 16 A direction in the xy-plane, starting at (x_0, y_0) and heading at an angle θ to the x-direction

In Figure 16, the arrow represents a direction in the xy-plane, and s is the distance travelled away from a starting point (x_0, y_0) in this direction. By simple trigonometry, we see that as we move away from (x_0, y_0), the x- and y-coordinates vary as

$$x = x_0 + s\cos\theta, \quad y = y_0 + s\sin\theta, \tag{26}$$

where θ is the (smaller) angle between the given direction and the positive x-direction. For a given direction, θ has a fixed value, so equations (26) define functions of the form $x = x(s)$ and $y = y(s)$. In other words, they are parametric equations describing a straight-line journey away from (x_0, y_0) in terms of the parameter s.

Substituting $x = x(s)$ and $y = y(s)$ in the function $f(x, y)$ gives a function $f(x(s), y(s))$ of s. We can therefore use the chain rule in the form of equation (23) to write down the rate of change of f with respect to s:

$$\frac{df}{ds} = \frac{\partial f}{\partial x}\frac{dx}{ds} + \frac{\partial f}{\partial y}\frac{dy}{ds}.$$

The derivatives dx/ds and dy/ds are immediately found from equations (26), so we conclude that

$$\frac{df}{ds} = \frac{\partial f}{\partial x}\cos\theta + \frac{\partial f}{\partial y}\sin\theta.$$

But what does df/ds mean? It is the rate of change of f, the height of the surface, with respect to the parameter s. In this case, however, the parameter s is the distance travelled in the chosen direction. It follows that at any given point, df/ds is the *slope of the surface in the chosen direction*.

We conclude that at a point (x, y), the slope of the surface $z = f(x, y)$ in a chosen direction is

$$\text{slope} = f_x(x, y)\cos\theta + f_y(x, y)\sin\theta, \tag{27}$$

where θ is related to the chosen direction as shown in Figure 16.

Rather than referring to Figure 16, it is convenient to specify our chosen direction more compactly. The unit vector in the chosen direction is just

$$\widehat{\mathbf{n}} = \cos\theta\,\mathbf{i} + \sin\theta\,\mathbf{j},$$

and this has components $\widehat{n}_x = \cos\theta$ and $\widehat{n}_y = \sin\theta$, so we can restate our conclusion as follows.

Slope of a surface in an arbitrary direction

At any point (x, y), the slope of the surface $z = f(x, y)$ in the direction of the unit vector $\widehat{\mathbf{n}}$ is

$$\text{slope in } \widehat{\mathbf{n}}\text{-direction} = \widehat{n}_x\, f_x(x, y) + \widehat{n}_y\, f_y(x, y). \tag{28}$$

We will rephrase and apply this result in the next subsection, using the important concept of *gradient*.

Exercise 13

Check that equation (28) makes sense in the following special cases.

(a) $\widehat{\mathbf{n}}$ points in the x-direction

(b) $\widehat{\mathbf{n}}$ points in the y-direction

2.4 The gradient vector and maximum slope

For a given surface $z = f(x, y)$, the slope at a given point depends on the direction chosen for $\widehat{\mathbf{n}}$. In one direction, the slope is greatest, and this corresponds to climbing straight up the hill. In another direction, the slope is zero, and this corresponds to skirting the hill, following a contour line.

To investigate the various slopes that can be obtained, it is very useful to define a new quantity. We take the first-order partial derivatives $f_x(x, y)$ and $f_y(x, y)$ and form the vector $f_x(x, y)\,\mathbf{i} + f_y(x, y)\,\mathbf{j}$. This is called the *gradient vector*, and is denoted by $\mathbf{grad}\, f$.

Note that **grad** is printed in bold because the gradient is a vector function. In your written work you should underline it.

The gradient vector

Given a function $f(x, y)$, the **gradient vector** or **gradient** of f is defined by

$$\mathbf{grad}\, f = f_x(x, y)\,\mathbf{i} + f_y(x, y)\,\mathbf{j} = \frac{\partial f}{\partial x}\,\mathbf{i} + \frac{\partial f}{\partial y}\,\mathbf{j}. \tag{29}$$

This is a vector-valued function of x and y. At a given point (a, b), it is a particular vector:

$$[\mathbf{grad}\, f]_{x=a,\, y=b} = f_x(a, b)\,\mathbf{i} + f_y(a, b)\,\mathbf{j}. \tag{30}$$

Exercise 14

Calculate the gradient of the function $f(x, y) = xy^2$, and evaluate it at the point $(1, 2)$.

According to definition (29), the components $[\mathbf{grad}\, f]_x$ and $[\mathbf{grad}\, f]_y$ of the gradient vector are just the first-order partial derivatives f_x and f_y, and this allows us to rewrite equation (28) as

$$\begin{aligned}\text{slope in } \widehat{\mathbf{n}}\text{-direction} &= \widehat{n}_x\,[\mathbf{grad}\, f]_x + \widehat{n}_y\,[\mathbf{grad}\, f]_y \\ &= \widehat{\mathbf{n}} \cdot \mathbf{grad}\, f. \end{aligned} \tag{31}$$

In this context, $[\mathbf{grad}\, f]_x$ and $[\mathbf{grad}\, f]_y$ are the x- and y-components of the vector $\mathbf{grad}\, f$.

The right-hand side is the scalar product of two vectors, $\widehat{\mathbf{n}}$ and $\mathbf{grad}\, f$.

Recall from Unit 4 that the component of a vector $\mathbf{a}$ in the direction of the unit vector $\widehat{\mathbf{n}}$ is given by the scalar product $\widehat{\mathbf{n}} \cdot \mathbf{a}$.

Because $\widehat{\mathbf{n}}$ is a unit vector, we can say that the slope in the direction of $\widehat{\mathbf{n}}$ is equal to the *component* of $\mathbf{grad}\, f$ in the direction of $\widehat{\mathbf{n}}$ – a simple and memorable result.

Example 8

Calculate the slope of the function $f(x, y) = xy^3$ at the point $(1, 2)$, in the direction of the unit vector $\widehat{\mathbf{n}} = \frac{3}{5}\,\mathbf{i} - \frac{4}{5}\,\mathbf{j}$.

Solution

The gradient of the function is

$$\mathbf{grad}\, f = \frac{\partial f}{\partial x}\,\mathbf{i} + \frac{\partial f}{\partial y}\,\mathbf{j} = y^3\,\mathbf{i} + 3xy^2\,\mathbf{j}.$$

At any point (x, y), the slope in the direction of the unit vector $\widehat{\mathbf{n}}$ is

$$\widehat{\mathbf{n}} \cdot \mathbf{grad}\, f = \left(\tfrac{3}{5}\,\mathbf{i} - \tfrac{4}{5}\,\mathbf{j}\right) \cdot \left(y^3\,\mathbf{i} + 3xy^2\,\mathbf{j}\right) = \tfrac{3}{5}y^3 - \tfrac{12}{5}xy^2,$$

so at the point $(1, 2)$, the slope is $24/5 - 48/5 = -24/5 = -4.8$.

Exercise 15

Calculate the slope of the function $f(x, y) = 2x^2y^2 + 3xy^3$ at the point $(1, 2)$, in the direction of the (non-unit) vector $\mathbf{i} - \mathbf{j}$.

A note on terminology

When dealing with the graph of a function of one variable, we use the words slope and gradient interchangeably. For a function of two variables, we must be more careful. We refer to the *slope* in a particular direction. The *gradient* is the gradient vector in equation (29). The component of the gradient in a given direction is equal to the slope in that direction, but the gradient vector is not itself a slope.

We can use the properties of scalar products to deduce some properties of the gradient vector. Any scalar product $\mathbf{a} \cdot \mathbf{b}$ can be written as $|\mathbf{a}|\,|\mathbf{b}| \cos\alpha$, where α is the (smaller) angle between the directions of $\mathbf{a}$ and $\mathbf{b}$. Since $\widehat{\mathbf{n}}$ is a unit vector, with $|\widehat{\mathbf{n}}| = 1$, equation (31) gives

$$\text{slope in } \widehat{\mathbf{n}}\text{-direction} = |\widehat{\mathbf{n}}|\,|\mathbf{grad}\, f| \cos\alpha = |\mathbf{grad}\, f| \cos\alpha, \qquad (32)$$

where α is the angle between the directions of $\widehat{\mathbf{n}}$ and $\mathbf{grad}\, f$. From this equation we can gather a rich harvest.

- The slope varies with α, and the maximum slope arises when $\cos\alpha = 1$ and $\alpha = 0$. This occurs when $\widehat{\mathbf{n}}$ points in the same direction as $\mathbf{grad}\, f$. So the maximum slope is found in the direction of the vector $\mathbf{grad}\, f$. Put another way, the direction of $\mathbf{grad}\, f$ has a simple interpretation: it is the direction of maximum slope.

- Setting $\alpha = 0$ in equation (32), the maximum slope is equal to $|\mathbf{grad}\, f|$. So the magnitude of $\mathbf{grad}\, f$ is equal to the maximum slope.
- Along a contour line, the function values are constant and the slope is zero. So if $\widehat{\mathbf{n}}$ points along a contour line of f, the slope must be equal to zero. However, equation (32) shows that zero slope corresponds to $\cos\alpha = 0$ and $\alpha = \pi/2$, which tells us that $\widehat{\mathbf{n}}$ and $\mathbf{grad}\, f$ are perpendicular. Hence $\mathbf{grad}\, f$ is perpendicular to the contour lines of f.

The properties of the gradient vector may be summarised as follows.

Properties of the gradient vector

For a smooth surface $z = f(x, y)$, at any given point (x, y):

- the gradient vector $\mathbf{grad}\, f$ is a vector in the xy-plane
- $\mathbf{grad}\, f$ points in the direction of maximum slope, and its magnitude is equal to the maximum slope
- $\mathbf{grad}\, f$ is perpendicular to the contour line at the given point.

To illustrate these properties, consider the function $f(x, y) = x^2 + y^2$, plotted in Figure 17(a). In this case, the gradient vector is

$$\mathbf{grad}\, f = 2x\,\mathbf{i} + 2y\,\mathbf{j},$$

and this defines a vector at each point in the xy-plane. Figure 17(b) shows arrows representing the gradient vectors at a selection of points.

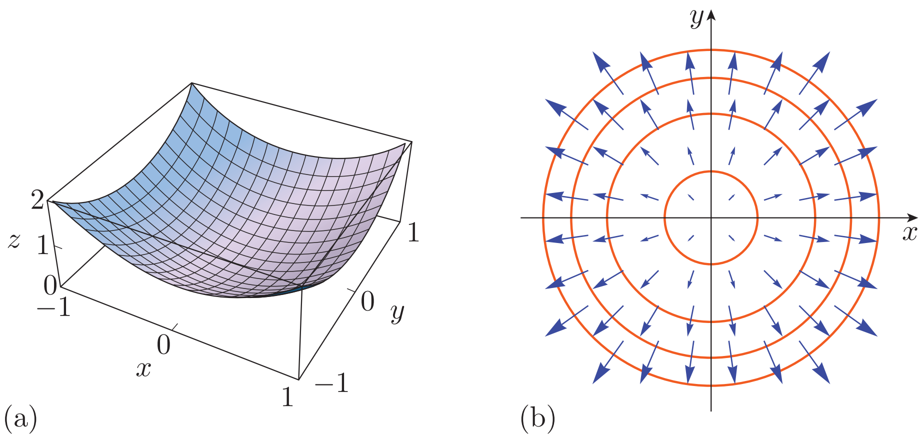


Figure 17 (a) A three-dimensional graph of $f(x, y) = x^2 + y^2$. (b) A map in the xy-plane with arrows representing $\mathbf{grad}\, f$ at a selection of points. Contour lines of $f(x, y)$ are shown in orange.

In this case, $\mathbf{grad}\, f$ points radially away from the origin, and its magnitude increases with radial distance from the origin. This makes sense because the slope is steepest in the radially outward direction, and the maximum slope grows as we move outwards. Figure 17(b) also plots the contour lines, which are circles centred on the origin. As expected, the contour line through any given point is perpendicular to the gradient vector at that point.

Exercise 16

Given a function $f(x,y)$, how would you characterise the direction in the xy-plane that gives the steepest *decrease* in $f(x,y)$ at a given point (a,b)?

Exercise 17

A bug in the xy-plane finds itself in a toxic environment. The level of toxicity is given by the function $f(x,y) = 2x^2y - 3x^3$. The bug is at the point $(1,2)$. In what direction away from $(1,2)$ should it initially move in order to lower its exposure to the toxin as rapidly as possible? Specify the direction as a unit vector.

2.5 The chain rule beyond two variables

So far we have focused on functions of two variables. For functions of three or more variables, it is really a case of 'more of the same thing'. For example, if $f = f(x,y,z)$, the chain rule for small changes becomes

$$\delta f = \frac{\partial f}{\partial x}\,\delta x + \frac{\partial f}{\partial y}\,\delta y + \frac{\partial f}{\partial z}\,\delta z.$$

This has the same pattern as for a function of two variables, but with an extra term involving z. The same is true for all the other forms of the chain rule. For example, if $x = x(t)$, $y = y(t)$ and $z = z(t)$, we have

$$\frac{df}{dt} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt} + \frac{\partial f}{\partial z}\frac{dz}{dt}.$$

The calculations get a bit longer, but are essentially the same.

For a function $f(x,y,z)$, the gradient vector is a vector in three-dimensional space, given by

$$\mathbf{grad}\, f = \frac{\partial f}{\partial x}\,\mathbf{i} + \frac{\partial f}{\partial y}\,\mathbf{j} + \frac{\partial f}{\partial z}\,\mathbf{k},$$

where $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are Cartesian unit vectors in three-dimensional space. At any given point, this gradient vector is perpendicular to the *contour surfaces* of $f(x,y,z)$ at that point. The direction of $\mathbf{grad}\, f$ is the direction in which the function increases most rapidly, and the magnitude of $\mathbf{grad}\, f$ is the maximum rate of change of f with respect to the distance moved in three-dimensional space.

Exercise 18

(a) Calculate the gradient of the function $f(x,y,z) = x^2 + y^2 + 2z^2$.

(b) The surface of a solid object is given by the equation $f(x,y,z) = 7$, where $f(x,y,z)$ is the function in part (a). Find a unit vector that is perpendicular to this surface at the point $(1,2,1)$.

Exercise 19

(a) Use the result of Example 3 to find the gradient of the function $V(x, y, z) = (x^2 + y^2 + z^2)^{-1/2}$.

(b) Describe in words the direction in which V increases most rapidly.

(c) What is the magnitude of $\mathbf{grad}\, V$ at any point $(x, y, z) \neq (0, 0, 0)$?

3 Taylor polynomials

This section is a sort of bridge. Our interest in Taylor polynomials arises mainly because they are needed in the final section of this unit, which deals with the stationary points of functions and their classification. The main point to grasp is the fact that close to a chosen point, functions can be approximated by polynomials. We start by revising the situation for functions of a single variable.

3.1 Review for functions of one variable

You know that a function of one variable can be approximated by a suitable polynomial. For example, Figure 18 shows that the function $f(x) = \sin x$ can be approximated near $x = 0$ by the simple polynomial $p(x) = x$. This approximation is a good one provided that we stay close enough to $x = 0$ (say within 0.1 of it). Similarly, Figure 19 shows that the function $g(x) = \cos x$ can be approximated near $x = \pi$ by the second-order polynomial $p(x) = -1 + \frac{1}{2}(x - \pi)^2$.

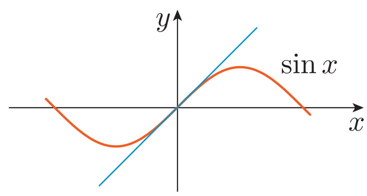


Figure 18 Near $x = 0$, $\sin x$ (orange) is approximated by $p(x) = x$ (blue)

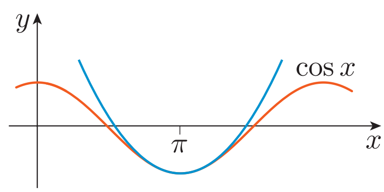


Figure 19 Near $x = \pi$, $\cos x$ (orange) is approximated by $p(x) = -1 + \frac{1}{2}(x - \pi)^2$ (blue)

How do we choose a suitable polynomial to use in any particular case? If we want to approximate the function $f(x)$ near the point $x = a$, the secret is to choose a polynomial that matches $f(x)$ in value, and in the values of its first few derivatives, at $x = a$.

For example, let us compare the function $f(x) = \sin x$ with the polynomial $p(x) = x$ at the point $x = 0$. The values match at $x = 0$ because $f(0) = p(0) = 0$. The first derivatives are

$$f'(x) = \cos x \quad \text{and} \quad p'(x) = 1.$$

These also match at $x = 0$ because $f'(0) = p'(0) = 1$. Finally, the second derivatives are

$$f''(x) = -\sin x \quad \text{and} \quad p''(x) = 0,$$

and these also match at $x = 0$ because $f''(0) = p''(0) = 0$.

Exercise 20

Show that the function $f(x) = \cos x$ and the polynomial $p(x) = -1 + \frac{1}{2}(x-\pi)^2$ are matched in their values and in the values of their first, second and third derivatives at $x = \pi$.

The problem of finding a suitable polynomial has a general solution. The polynomial that matches $f(x)$ in its values, and in the values of its first n derivatives, at the point $x = a$, is

$$\begin{aligned} p(x) = f(a) + f'(a)(x-a) + \frac{1}{2!}f''(a)(x-a)^2 \\ + \frac{1}{3!}f'''(a)(x-a)^3 + \cdots + \frac{1}{n!}f^{(n)}(a)(x-a)^n, \end{aligned} \tag{33}$$

where $f^{(n)}(a)$ is the nth derivative of $f(x)$ evaluated at $x = a$, and $n!$ is factorial n given by $n! = n(n-1)(n-2)\ldots 1$.

This polynomial is called the nth-order **Taylor polynomial** for $f(x)$ about $x = a$.

To take a definite case, consider the function $f(x) = \cos x$ of Exercise 20. In this case, successive differentiations give

$$f(x) = \cos x, \quad f'(x) = -\sin x, \quad f''(x) = -\cos x, \quad f'''(x) = \sin x.$$

So at the point $x = \pi$, we have

$$f(\pi) = -1, \quad f'(\pi) = 0, \quad f''(\pi) = 1, \quad f'''(\pi) = 0.$$

Substituting these constants into equation (33) gives the third-order Taylor polynomial for $\cos x$ about the point $x = \pi$:

$$p(x) = -1 + \tfrac{1}{2}(x-\pi)^2,$$

and this is just what we used in Figure 19.

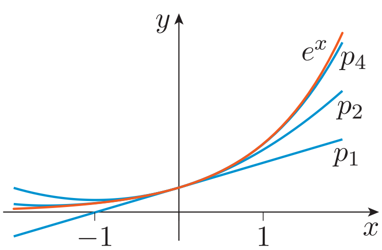


Figure 20 A graph of e^x against x (in orange) compared with Taylor polynomials for e^x of orders 1, 2 and 4 (blue)

Two points about Taylor polynomials are worth mentioning. First, for many functions, higher-order Taylor polynomials produce successively better approximations. This is illustrated in Figure 20. Second, as we approach the point $x = a$ about which a given low-order Taylor polynomial is calculated, the polynomial becomes increasingly accurate. If we get *extremely* close to the point $x = a$, the function and its low-order Taylor polynomials become practically indistinguishable.

Exercise 21

(a) Find the first and second derivatives of the function $f(t) = \ln(1+t^2)$.

(b) Write down the second-order Taylor polynomial for $f(t)$ about the point $t = 0$.

(c) Write down the second-order Taylor polynomial for $f(t)$ about the point $t = 1$.

3.2 Functions of two variables

We now extend the concept of a Taylor polynomial to functions of two or more variables. First we must generalise the idea of a polynomial to cover more than one variable. An expression of the form

$$p(x,y) = A + Bx + Cy, \tag{34}$$

where A, B and C are constants (with B and C not both equal to zero), is called a polynomial of order 1 in x and y. It is also called a *linear polynomial* in x and y.

Polynomials in more than one variable are also called *multinomials*.

An expression of the form

$$p(x,y) = A + Bx + Cy + Dx^2 + Exy + Fy^2, \tag{35}$$

where A, B, C, D, E and F are constants (with D, E and F not all equal to zero), is called a polynomial of order 2. It is also called a *quadratic polynomial* in x and y.

Notice that each term in these polynomials is of the form constant $\times\, x^n y^m$, where n and m are zero or positive integers. A term in a polynomial is said to be of order N if $n + m = N$. So linear polynomials contain terms up to order 1, and quadratic polynomials contain terms up to order 2.

Given a function $f(x,y)$, we would like to find a suitable polynomial in x and y that approximates the function in the vicinity of a point (a,b). The key is to choose the coefficients in the polynomial in such a way that the function and the polynomial match in their values, and in the values of their first n partial derivatives, at the point (a,b). This is just what an nth-order Taylor polynomial does. In practice, we need Taylor polynomials of only first and second order, so we will concentrate on these.

We will first write down a general expression for the first-order Taylor polynomial for a function $f(x,y)$ about a point (a,b). Then we will check that it has the desired properties. This process will then be repeated for the second-order Taylor polynomial.

First-order Taylor polynomial

The **first-order Taylor polynomial** for $f(x,y)$ about (a,b) is

$$p_1(x,y) = f(a,b) + f_x(a,b)(x-a) + f_y(a,b)(y-b). \tag{36}$$

We can easily check that this polynomial does what is needed. Setting $x = a$ and $y = b$ in equation (36), we see that $p_1(a,b) = f(a,b)$, so the function and the polynomial have the same value at the point (a,b). Moreover, a and b have fixed values, so $f(a,b)$, $f_x(a,b)$ and $f_y(a,b)$ are all constants. Partial differentiation of $p_1(x,y)$ with respect to x and y then gives

$$\frac{\partial p_1}{\partial x} = f_x(a,b) = \left.\frac{\partial f}{\partial x}\right|_{x=a,\,y=b} \quad\text{and}\quad \frac{\partial p_1}{\partial y} = f_y(a,b) = \left.\frac{\partial f}{\partial y}\right|_{x=a,\,y=b}.$$

In particular, the values of $\partial p_1/\partial x$ and $\partial p_1/\partial y$ match those of $\partial f/\partial x$ and $\partial f/\partial y$ at (a,b), so the function and the polynomial $p_1(x,y)$ are matched in their values, and in the values of their *first-order* partial derivatives, at the point (a,b). This is what is required of a first-order Taylor polynomial.

The second-order Taylor polynomial for a function involves its second-order partial derivatives.

Be careful to get the second line right: common errors are to not multiply all three terms by $\frac{1}{2}$, or to omit the factor 2 in the middle term.

Second-order Taylor polynomial

The **second-order Taylor polynomial** for $f(x,y)$ about (a,b) is

$$\begin{aligned}p_2(x,y) = f(a,b) &+ f_x(a,b)(x-a) + f_y(a,b)(y-b)\\ &+ \tfrac{1}{2}\big(f_{xx}(a,b)(x-a)^2 + 2f_{xy}(a,b)(x-a)(y-b)\\ &\qquad + f_{yy}(a,b)(y-b)^2\big).\end{aligned} \tag{37}$$

It is straightforward to check that the value of this polynomial, and the values of all its first- and second-order derivatives, match those of $f(x,y)$ at (a,b). This is done in the following exercise.

Exercise 22

Writing $h(x,y) = p_2(x,y)$, use equation (37) to show that

$$\begin{aligned}&h(a,b) = f(a,b),\\ &h_x(a,b) = f_x(a,b), \quad h_y(a,b) = f_y(a,b),\\ &h_{xx}(a,b) = f_{xx}(a,b), \quad h_{yy}(a,b) = f_{yy}(a,b), \quad h_{xy}(a,b) = f_{xy}(a,b).\end{aligned}$$

(There is no need to check that $h_{yx}(a,b) = f_{yx}(a,b)$ because this follows from $h_{xy}(a,b) = f_{xy}(a,b)$, thanks to the mixed partial derivative theorem.)

Example 9

Determine the Taylor polynomials of orders 1 and 2 about the point $(2,1)$ for the function $f(x,y) = x^3 + xy - 2y^2$.

Solution

Differentiating the function partially with respect to x and partially with respect to y gives

$$f_x(x,y) = 3x^2 + y, \quad f_y(x,y) = x - 4y.$$

Differentiating partially again gives

$$f_{xx}(x,y) = 6x, \quad f_{xy}(x,y) = 1, \quad f_{yy}(x,y) = -4.$$

It follows that

$$\begin{aligned}&f(2,1) = 8, \quad f_x(2,1) = 13, \quad f_y(2,1) = -2,\\ &f_{xx}(2,1) = 12, \quad f_{xy}(2,1) = 1, \quad f_{yy}(2,1) = -4,\end{aligned}$$

so the first-order Taylor polynomial is

$$p_1(x,y) = 8 + 13(x-2) - 2(y-1),$$

and the second-order Taylor polynomial is

$$\begin{aligned} p_2(x,y) &= 8 + 13(x-2) - 2(y-1) \\ &\qquad + \tfrac{1}{2}\big(12(x-2)^2 + 2(x-2)(y-1) - 4(y-1)^2\big) \\ &= 8 + 13(x-2) - 2(y-1) \\ &\qquad + 6(x-2)^2 + (x-2)(y-1) - 2(y-1)^2. \end{aligned}$$

The answer can be left in this form as, for many purposes, there is no advantage to be gained in collecting terms in powers of x and y.

Exercise 23

Given $f(x,y) = x^2e^{3y}$, find the first- and second-order Taylor polynomials for $f(x,y)$ about the point $(2,0)$.

The tangent plane

You saw in Subsection 1.3 that a function $f(x,y)$ can be plotted as a surface $z = f(x,y)$ in three-dimensional space. The first-order Taylor polynomial for this function is

$$p_1(x,y) = f(a,b) + f_x(a,b)(x-a) + f_y(a,b)(y-b),$$

and this can also be plotted as a surface

$$z = p_1(x,y).$$

Comparing with equation (3) and the discussion following it, we see that the surface $z = p_1(x,y)$ is a plane. It is called the **tangent plane** of the surface $z = f(x,y)$.

To see why this name is appropriate, first note that $f(a,b) = p_1(a,b)$, so the surface $z = f(x,y)$ coincides with the tangent plane at the point (a,b). We also know that the first partial derivatives of f are the same as those of p_1 at the point (a,b). So we must have

$$[\mathbf{grad}\, p_1]_{x=a,\, y=b} = f_x(a,b)\,\mathbf{i} + f_y(a,b)\,\mathbf{j} = [\mathbf{grad}\, f]_{x=a,\, y=b}. \qquad (38)$$

The slope in any chosen direction in the xy-plane is the component of the gradient vector in that direction, so *the tangent plane and the surface of the function have exactly the same slopes at (a,b) in all directions*. This is why the tangent plane is so-called. It is a natural generalisation of the concept of a tangent line to a curve at a given point (see Figure 21).

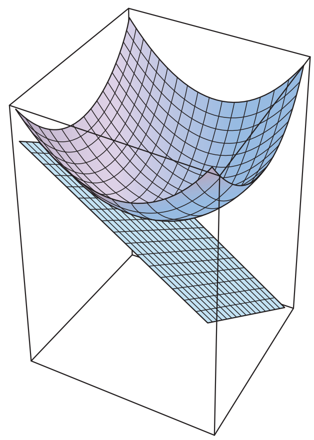


Figure 21 The tangent plane of $f(x,y) = x^2 + y^2$ at the point $x=-1$, $y=-1$

3.3 Matrix representation of Taylor polynomials

Our main interest will be in first- and second-order Taylor polynomials for functions of two or more variables. For future use, it will be helpful to take another look at equations (36) and (37), and recast them in matrix form.

First note that the first-order Taylor polynomial about (a,b) can be written as

$$\begin{aligned} p_1(x,y) &= f(a,b) + f_x(a,b)(x-a) + f_y(a,b)(y-b) \\ &= f(a,b) + \begin{bmatrix} f_x(a,b) & f_y(a,b) \end{bmatrix} \begin{bmatrix} x-a \\ y-b \end{bmatrix}. \end{aligned} \tag{39}$$

By using matrix multiplication on the right-hand side, you can check that this is equivalent to equation (36).

It is convenient to introduce the column vector

$$\mathbf{R} = \begin{bmatrix} x-a \\ y-b \end{bmatrix}, \tag{40}$$

which represents the displacement of the point (x,y) from (a,b) and is called the **displacement vector**. We also define

$$\mathbf{G} = \begin{bmatrix} f_x(a,b) \\ f_y(a,b) \end{bmatrix}, \tag{41}$$

which is a matrix representation of the **gradient vector**.

In terms of these matrices, the first-order Taylor polynomial can be written in the compact form

$$p_1(x,y) = f(a,b) + \mathbf{G}^T\mathbf{R}, \tag{42}$$

where the transpose converts the column matrix $\mathbf{G}$ into the row matrix needed in equation (39).

The second-order Taylor polynomial can also be written in matrix form. We introduce the matrix of second-order partial derivatives

$$\mathbf{H} = \begin{bmatrix} f_{xx}(a,b) & f_{xy}(a,b) \\ f_{yx}(a,b) & f_{yy}(a,b) \end{bmatrix}.$$

Then, using matrix multiplication, you can check that

$$\begin{aligned} \mathbf{R}^T\mathbf{H}\,\mathbf{R} &= \begin{bmatrix} x-a & y-b \end{bmatrix} \begin{bmatrix} f_{xx}(a,b) & f_{xy}(a,b) \\ f_{yx}(a,b) & f_{yy}(a,b) \end{bmatrix} \begin{bmatrix} x-a \\ y-b \end{bmatrix} \\ &= \begin{bmatrix} x-a & y-b \end{bmatrix} \begin{bmatrix} f_{xx}(a,b)(x-a) + f_{xy}(a,b)(y-b) \\ f_{yx}(a,b)(x-a) + f_{yy}(a,b)(y-b) \end{bmatrix} \\ &= f_{xx}(a,b)(x-a)^2 + 2f_{xy}(a,b)(x-a)(y-b) + f_{yy}(a,b)(y-b)^2, \end{aligned} \tag{43}$$

where we have used the mixed partial derivative theorem in the last step. Comparing with equation (37), we see that the second-order Taylor polynomial can be written as follows.

Second-order Taylor polynomial in matrix form

$$p_2(x,y) = f(a,b) + \mathbf{G}^T\mathbf{R} + \tfrac{1}{2}\mathbf{R}^T\mathbf{H}\,\mathbf{R}. \tag{44}$$

A compact formula is all well and good – but you might think that we would need to expand it out to use it. However, in the next section you will see that matrix methods can be applied directly to equation (44) to obtain useful results. In particular, the matrix $\mathbf{H}$ will become a focus of

attention. This matrix is called the **Hessian matrix** after the German mathematician Otto Hesse (1811–1874).

Equation (44) is also useful if we need a second-order Taylor polynomial for a function of three (or more) variables. This is because it remains true no matter how many variables the function contains! The only thing that changes is the size of the matrices **R**, **G** and **H**. For a function $f(x, y, z)$ of three variables, expanded about the point (a, b, c),

$$\mathbf{G} = \begin{bmatrix} f_x(a,b,c) \\ f_y(a,b,c) \\ f_z(a,b,c) \end{bmatrix} \quad \text{and} \quad \mathbf{R} = \begin{bmatrix} x-a \\ y-b \\ z-c \end{bmatrix},$$

while the Hessian matrix of second-order partial derivatives becomes

$$\mathbf{H} = \begin{bmatrix} f_{xx}(a,b,c) & f_{xy}(a,b,c) & f_{xz}(a,b,c) \\ f_{yx}(a,b,c) & f_{yy}(a,b,c) & f_{yz}(a,b,c) \\ f_{zx}(a,b,c) & f_{zy}(a,b,c) & f_{zz}(a,b,c) \end{bmatrix}.$$

You need not bother to multiply out these matrices because when we use equation (44) in the next section, we will need only some very general properties of its constituent matrices.

4 Minima, maxima and saddle points

A very useful aspect of calculus is that it gives us a way of finding the maximum or minimum values of a function, and it lets us find the conditions under which these maxima or minima are attained. In this final section you will see how maxima, minima and other stationary points are found and classified for functions of two or more variables.

Maxima and minima in the natural world

In the natural world, many phenomena are governed by maxima or minima. For example, a mechanical system reaches a condition of stable equilibrium when a quantity known as the *potential energy* reaches its minimum value: a chain suspended between two fixed points will hang in such a way that its potential energy is as small as possible (Figure 22). More complicated systems, that can exchange heat with their surroundings, reach a state of thermal and mechanical equilibrium when a quantity called the *free energy* is minimised. The folding of protein molecules, which determines their biological function, is dictated by the configurations of locally minimum free energy (Figure 23). Even systems in motion, such as planets orbiting the Sun, move in such a way that a quantity called the *action* is minimised. No wonder the great Euler, seeking an ultimate explanation, speculated:

> For since the fabric of the universe is most perfect and the work of a most wise Creator, nothing at all takes place in the universe in which some rule of maximum or minimum does not appear.

Figure 22 A chain hangs in such a way that its potential energy has a minimum value

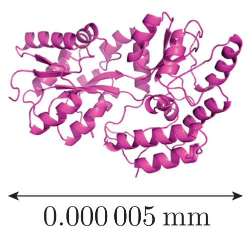


Figure 23 A protein molecule folds in such a way that its free energy has a local minimum value

4.1 Review for functions of one variable

To put our discussion in context, we will briefly remind you of the situation for functions of one variable. The main point is that functions can have local minima and local maxima.

If we are given a function $f(x)$ and a point $x = a$ inside its domain:

- a **local minimum** occurs at $x = a$ if there is a small region around a within which $f(x) > f(a)$ at all points $x \neq a$
- a **local maximum** occurs at $x = a$ if there is a small region around a within which $f(x) < f(a)$ at all points $x \neq a$
- there is an **extremum** at $x = a$ if this point is *either* a local maximum *or* a local minimum.

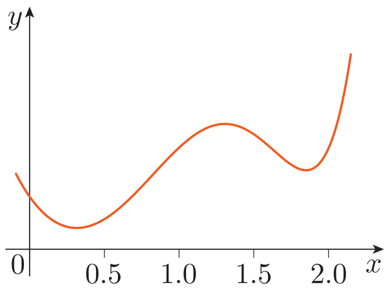


Figure 24 A function $y = f(x)$ with local minima and maxima

For example, the function in Figure 24 has local minima at $x = 0.3$ and $x = 1.8$, and a local maximum at $x = 1.3$. All these points are extrema.

There may be several local minima and maxima, so a particular local minimum need not give the smallest possible value of a function (the **global minimum**). Similarly, a particular local maximum need not give the largest possible value of a function (the **global maximum**). The global minimum and global maximum can be found by sifting through all the local minima and maxima. For example, the global minimum of the function in Figure 24 in the region $0 \leq x \leq 2$ is at $x = 0.3$. We will not discuss this point further, but concentrate on the task of finding the local minima and maxima.

We restrict attention to smooth functions $f(x)$, and ignore any minima or maxima that might occur on the boundaries of the domain of $f(x)$. Then calculus can help us to find the local minima and maxima. This is because the tangent line to the graph of $f(x)$ against x is horizontal at a local minimum or maximum. Equivalently, $df/dx = 0$ at such a point. Any point at which the first derivative df/dx is equal to zero is called a **stationary point**. So the extrema (i.e. the local minima and local maxima) are stationary points. However, we can also have stationary points that are not extrema.

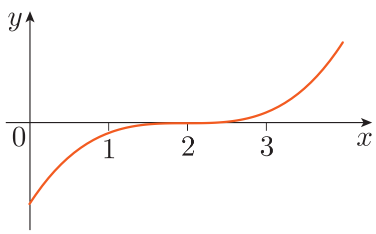


Figure 25 A function $y = f(x)$ with a horizontal point of inflection at $x = 2$

In Figure 25, the stationary point at $x = 2$ is neither a local maximum nor a local minimum. In the immediate vicinity of $x = 2$, points with $x < 2$ have smaller values than $f(2)$, while points with $x > 2$ have larger values than $f(2)$. Such a point is called a **horizontal point of inflection**.

We often need to classify the stationary points – that is, decide whether they are local minima, local maxima or points of inflection. To classify a stationary point at $x = a$, it is helpful to use the second-order Taylor polynomial for $f(x)$ about a:

$$p_2(x) = f(a) + f'(a)(x-a) + \frac{1}{2!}f''(a)(x-a)^2.$$

Since a is a stationary point, we know (by definition) that $f'(a) = 0$, so

$$f(x) \simeq p_2(x) = f(a) + \frac{1}{2!}f''(a)(x-a)^2 \quad \text{(for } x \text{ close to } a\text{).} \tag{45}$$

Now, if we consider a small enough region around $x = a$, then the second-order Taylor polynomial $p_2(x)$ will approximate $f(x)$ extremely well – so well, that we can replace the above $\simeq$ sign by an equals sign with negligible error. Then looking at equation (45), we see that the condition $f''(a) > 0$ guarantees that $f(x) > f(a)$ for all points $x \neq a$. This is precisely the definition of a local minimum. A similar argument, but with $f''(a) < 0$, leads to a local maximum. We therefore have the following test.

Second derivative test for stationary points

Given a function $f(x)$, we can say that:

- when $f'(a) = 0$ and $f''(a) > 0$, we have a local minimum at $x = a$
- when $f'(a) = 0$ and $f''(a) < 0$, we have a local maximum at $x = a$.

The test works unless $f''(a) = 0$, in which case the test gives us no information; we would need to look at higher-order Taylor polynomials to make a decision. Also note that the second derivative test never identifies a horizontal point of inflection. This is not a great problem because in practical cases the main interest lies in minima and maxima.

4.2 Stationary points for functions of two variables

We will now try to extend the above ideas to a smooth function $f(x, y)$ of two variables. The definitions of local minima and local maxima are essentially the same as before, but take account of the fact that points and regions are now specified by two coordinates.

Local minima and maxima

Given a function $f(x, y)$ and a point (a, b) inside the domain of f:

- a **local minimum** occurs at (a, b) if there is a small region around (a, b) within which $f(x, y) > f(a, b)$ at all points $(x, y) \neq (a, b)$
- a **local maximum** occurs at (a, b) if there is a small region around (a, b) within which $f(x, y) < f(a, b)$ at all points $(x, y) \neq (a, b)$.

Here, 'inside' implies not on any boundary line.

As before, an **extremum** is a point that is *either* a local minimum *or* a local maximum. For a smooth function $f(x, y)$, the tangent plane to the surface $z = f(x, y)$ is horizontal at any extremum. This means that the slope of the tangent plane is equal to zero for any direction in the xy-plane, so both the partial derivatives f_x and f_y must be zero at an extremum.

Stationary points

A point (a,b) is a **stationary point** of a function $f(x,y)$ if both $f_x(a,b)$ and $f_y(a,b)$ are equal to zero.

All extrema (i.e. all local minima and maxima) are stationary points, but some stationary points are not extrema. Figure 26 shows the three cases that can occur. In all three cases, there is a stationary point at $(0,0)$ because both the partial derivatives f_x and f_y are equal to zero there.

In Figure 26(a), we have a local minimum because all paths moving smoothly away from $(0,0)$ initially climb upwards to higher function values. In Figure 26(b), we have a local maximum because all paths moving smoothly away from $(0,0)$ initially descend downwards to lower function values. But in Figure 26(c), we have something different: some paths moving away from $(0,0)$ climb upwards, and others descend downwards. This stationary point is neither a local minimum nor a local maximum. It is called a *saddle point* because the shape of the surface is rather like the shape of a saddle placed on a horse's back.

Saddle points

A **saddle point** is a stationary point that is neither a local minimum nor a local maximum. Through such a point, some paths climb to higher function values, while others descend to lower function values.

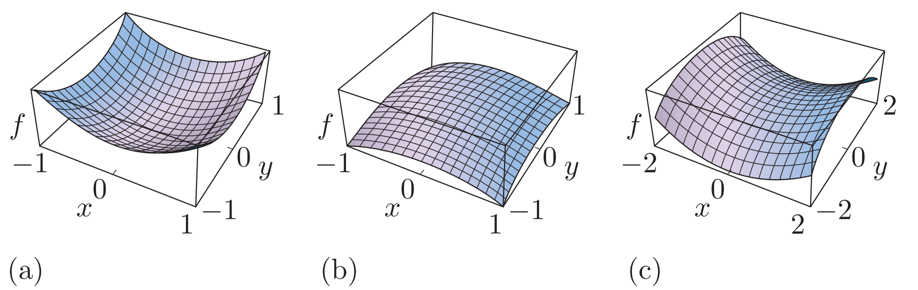


Figure 26 Functions with stationary points at $(0,0)$: (a) a local minimum; (b) a local maximum; (c) a saddle point

In the next subsection you will see how stationary points can be classified using second-order partial derivatives. For the moment, we concentrate on locating the stationary points using first-order partial derivatives.

Example 10

Locate the stationary point(s) of the function

$$f(x,y) = x^2 + y^2 + (x-1)(y+2).$$

Solution

Partially differentiating with respect to x gives

$$f_x(x, y) = 2x + y + 2,$$

and partially differentiating with respect to y gives

$$f_y(x, y) = 2y + x - 1.$$

At a stationary point, $f_x = f_y = 0$, so we need to solve the pair of simultaneous equations

$$\begin{aligned} 2x + y &= -2, \\ x + 2y &= 1. \end{aligned}$$

These equations have the solution $x = -5/3$, $y = 4/3$, so the only stationary point is at $(x, y) = (-5/3, 4/3)$.

A note of caution! We can always carry out the partial differentiations needed to obtain the simultaneous equations $f_x = 0$, $f_y = 0$. In this unit, such equations can always be solved by hand. More generally, however, the equations may be too complicated for this – they would then be solved numerically on a computer.

Exercise 24

Locate the stationary point(s) of the function

$$f(x, y) = 3x^2 - 4xy + 2y^2 + 4x - 8y.$$

Exercise 25

Locate the stationary point(s) of the function

$$f(x, y) = xy(x + y - 3).$$

4.3 The eigenvalue test

There remains the task of classifying the stationary points – deciding which are local maxima, which are local minima, and which are saddle points. In broad terms, our tactics will be the same as for functions of a single variable: we will use the second-order Taylor polynomial. This method works for functions of any number of variables, but we will initially consider a function $f(x, y)$ of two variables.

Suppose that $f(x, y)$ has a stationary point at (a, b), and that $p_2(x, y)$ is the second-order Taylor polynomial for $f(x, y)$ about (a, b). The full expression for this polynomial is given in equation (37), but there are great advantages in using the matrix version given in equation (44).

This is

$$p_2(x,y) = f(a,b) + \mathbf{G}^T\mathbf{R} + \tfrac{1}{2}\mathbf{R}^T\mathbf{H}\,\mathbf{R}, \tag{46}$$

where

$$\mathbf{G} = \begin{bmatrix} f_x(a,b) \\ f_y(a,b) \end{bmatrix} \quad \text{and} \quad \mathbf{R} = \begin{bmatrix} x-a \\ y-b \end{bmatrix}$$

are the gradient at (a,b) and the displacement away from (a,b), written as column vectors, and $\mathbf{H}$ is the Hessian matrix of second derivatives at (a,b):

$$\mathbf{H} = \begin{bmatrix} f_{xx}(a,b) & f_{xy}(a,b) \\ f_{yx}(a,b) & f_{yy}(a,b) \end{bmatrix}.$$

Because (a,b) is a stationary point, both $f_x(a,b)$ and $f_y(a,b)$ are equal to zero. The gradient matrix $\mathbf{G}$ therefore has both elements equal to zero, and equation (46) reduces to

$$p_2(x,y) = f(a,b) + \tfrac{1}{2}\mathbf{R}^T\mathbf{H}\,\mathbf{R}.$$

In the immediate vicinity of (a,b), any small difference between $f(x,y)$ and $p_2(x,y)$ becomes negligible, and we can safely replace $p_2(x,y)$ on the left-hand side by $f(x,y)$. Rearranging slightly, we can write

$$f(x,y) - f(a,b) = \tfrac{1}{2}\mathbf{R}^T\mathbf{H}\,\mathbf{R}, \tag{47}$$

provided that (x,y) is close enough to the stationary point at (a,b).

Multiplying out the matrix product on the right-hand side of equation (47), it is easy to see that

This matrix multiplication was carried out in equation (43).

$$\begin{aligned}\mathbf{R}^T\mathbf{H}\,\mathbf{R} = {} & f_{xx}(a,b)(x-a)^2 + f_{yy}(a,b)(y-b)^2 \\ & + 2f_{xy}(a,b)(x-a)(y-b).\end{aligned} \tag{48}$$

Denoting the right-hand side of this equation by $Q(x,y)$, we can write

$$\mathbf{R}^T\mathbf{H}\,\mathbf{R} = Q(x,y), \tag{49}$$

where $Q(x,y)$ is a quadratic function of x and y with coefficients that depend on the second-order partial derivatives of $f(x,y)$ at the stationary point (a,b).

Now, recall how local minima, local maxima and saddle points are defined.

For a *local minimum*, the function values all around the stationary point are greater than at the stationary point itself. This means that $f(x,y) > f(a,b)$ for all (x,y) that are sufficiently close, but not equal, to (a,b). Using equations (47) and (49), we see that this condition is guaranteed if $Q(x,y) > 0$ for all $(x,y) \neq (a,b)$.

For a *local maximum*, the function values all around the stationary point are smaller than at the stationary point itself. This is guaranteed if $Q(x,y) < 0$ for all $(x,y) \neq (a,b)$.

Saddle points correspond to increases in some directions and decreases in others, so the sign of $Q(x,y)$ must depend on x and y in this case. We therefore have the following criterion.

The nature of a stationary point (a, b) depends on $Q(x, y) = \mathbf{R}^T \mathbf{H}\,\mathbf{R}$.

- If $Q(x, y) > 0$ for all $(x, y) \neq (a, b)$, then we have a local minimum.
- If $Q(x, y) < 0$ for all $(x, y) \neq (a, b)$, then we have a local maximum.
- If $Q(x, y)$ is positive for some (x, y) and negative for other (x, y), then we have a saddle point.

Given any function $f(x, y)$ with a stationary point at (a, b), we can try to classify this stationary point by examining the sign of $Q(x, y)$ for all x and y around (a, b). Let us take a very simple example. Suppose that

$$f(x, y) = (x - 1)^2 + (y - 1)^2.$$

Then

$$f_x = 2(x - 1) \quad \text{and} \quad f_y = 2(y - 1),$$

so there is a stationary point at $(1, 1)$. The second-order partial derivatives are

$$f_{xx} = 2, \quad f_{yy} = 2, \quad f_{xy} = f_{yx} = 0,$$

which are constants in this case. Hence equation (48) gives

$$Q(x, y) = 2(x - 1)^2 + 2(y - 1)^2.$$

This the sum of two squared terms, neither of which can be negative, so $Q(x, y) > 0$ for all $(x, y) \neq (1, 1)$. We therefore conclude that the stationary point $(1, 1)$ is a local minimum. This is hardly surprising, but illustrates the logic of our method.

Using eigenvalues

In a more general case, the sign of Q may not be so obvious. Fortunately, there is a systematic way to proceed, using the eigenvalues of the Hessian matrix $\mathbf{H}$. The method hinges on the fact that $\mathbf{H}$ is a real symmetric matrix. It is real because f, x and y are all real-valued, so f_{xx}, f_{yy}, f_{xy} and f_{yx} are all real. And it is symmetric because the mixed partial derivative theorem ensures that $f_{xy} = f_{yx}$.

You know from Unit 5 that real symmetric matrices have some special properties. Their eigenvalues are always real, and their eigenvectors can always be chosen to be real, of unit magnitude and mutually orthogonal. For the 2×2 Hessian matrix considered here, there are two real eigenvalues λ_1 and λ_2, corresponding to two real orthogonal eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$, so

$$\mathbf{H}\mathbf{v}_1 = \lambda_1 \mathbf{v}_1 \quad \text{and} \quad \mathbf{H}\mathbf{v}_2 = \lambda_2 \mathbf{v}_2. \tag{50}$$

The displacement vector $\mathbf{R}$ can be written as a linear combination of the two real orthogonal eigenvectors:

$$\mathbf{R} = \alpha \mathbf{v}_1 + \beta \mathbf{v}_2,$$

where the components α and β are real (because $\mathbf{R}$, $\mathbf{v}_1$ and $\mathbf{v}_2$ are real).

$\mathbf{R}$, α and β are functions of x and y.

Applying $\mathbf{H}$ to $\mathbf{R}$, and using the eigenvalue equations (50), we get

$$\mathbf{H}\,\mathbf{R} = \mathbf{H}(\alpha\mathbf{v}_1 + \beta\mathbf{v}_2) = \alpha(\mathbf{H}\mathbf{v}_1) + \beta(\mathbf{H}\mathbf{v}_2) = \alpha\lambda_1\mathbf{v}_1 + \beta\lambda_2\mathbf{v}_2.$$

We also have

$$\mathbf{R}^T = \alpha\mathbf{v}_1^T + \beta\mathbf{v}_2^T,$$

so

$$Q(x,y) = \mathbf{R}^T\mathbf{H}\,\mathbf{R} = (\alpha\mathbf{v}_1^T + \beta\mathbf{v}_2^T)(\alpha\lambda_1\mathbf{v}_1 + \beta\lambda_2\mathbf{v}_2). \tag{51}$$

Finally, we use the fact that $\mathbf{v}_1$ and $\mathbf{v}_2$ are of unit magnitude and mutually orthogonal. In matrix terms, this means that

$$\mathbf{v}_1^T\mathbf{v}_1 = 1, \quad \mathbf{v}_2^T\mathbf{v}_2 = 1, \quad \mathbf{v}_1^T\mathbf{v}_2 = 0, \quad \mathbf{v}_2^T\mathbf{v}_1 = 0.$$

So multiplying out the brackets in equation (51) gives

$$Q(x,y) = \alpha^2\lambda_1 + \beta^2\lambda_2, \tag{52}$$

where α and β vary over a range of real values as x and y vary. Away from the stationary point, the displacement vector $\mathbf{R}$ is non-zero, which means that the components α and β cannot simultaneously be equal to zero. You have already seen that the nature of the stationary point is determined by the sign of $Q(x,y)$. Now we see that this is determined by the signs of the eigenvalues λ_1 and λ_2 of $\mathbf{H}$.

- When both eigenvalues are positive, $Q(x,y) > 0$, and the stationary point is a local minimum.
- When both eigenvalues are negative, $Q(x,y) < 0$, and the stationary point is a local minimum.
- When the eigenvalues have opposite signs, $Q(x,y)$ may be positive or negative, and the stationary point is a saddle point.

This leads to the following procedure.

Procedure 1 The eigenvalue test

Suppose that we are given a smooth function $f(x,y)$ with a stationary point at (a,b). To establish the nature of the stationary point, do the following.

1. Find the second-order partial derivatives, and evaluate them at the stationary point.
2. Construct the Hessian matrix $\mathbf{H}$ at the stationary point, and determine its eigenvalues.
3. Apply the following rules:
   - If all the eigenvalues are positive, we have a local minimum.
   - If all the eigenvalues are negative, we have a local maximum.
   - If the eigenvalues have mixed signs, we have a saddle point.

This procedure does not cover the case where the eigenvalues do not have mixed signs but include a zero; in this case, the test is inconclusive.

Example 11

Locate the stationary point(s) of the function $f(x, y) = e^{-(x^2+y^2)}$, and use the eigenvalue test to classify them.

Solution

Partial differentiation gives

$$f_x = -2xe^{-(x^2+y^2)} \quad \text{and} \quad f_y = -2ye^{-(x^2+y^2)}.$$

Since $f_x = 0$ only when $x = 0$, and $f_y = 0$ only when $y = 0$, there is a single stationary point, at $(0, 0)$.

The second-order partial derivatives are

$$\begin{aligned} f_{xx} &= -2e^{-(x^2+y^2)} + 4x^2e^{-(x^2+y^2)}, \\ f_{yy} &= -2e^{-(x^2+y^2)} + 4y^2e^{-(x^2+y^2)}, \\ f_{xy} &= 4xye^{-(x^2+y^2)}. \end{aligned}$$

At the stationary point $(0, 0)$, we have $f_{xx}(0, 0) = -2$, $f_{yy}(0, 0) = -2$ and $f_{xy}(0, 0) = 0$. So the Hessian matrix at $(0, 0)$ is

$$\mathbf{H} = \begin{bmatrix} f_{xx}(0,0) & f_{xy}(0,0) \\ f_{yx}(0,0) & f_{yy}(0,0) \end{bmatrix} = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix}.$$

The eigenvalues satisfy

$$0 = \det(\mathbf{H} - \lambda\mathbf{I}) = \begin{vmatrix} -2-\lambda & 0 \\ 0 & -2-\lambda \end{vmatrix} = (2+\lambda)^2,$$

so they are $\lambda_1 = -2$ and $\lambda_2 = -2$. These are both negative, so the stationary point $(0, 0)$ is a local maximum.

For a diagonal matrix, the eigenvalues are equal to the diagonal matrix elements.

Exercise 26

Locate and classify the stationary point of the function

$$f(x, y) = 2x^2 - xy - 3y^2 - 3x + 7y.$$

A minor shortcut is available for functions of two variables. You may recall from Unit 5 that the eigenvalues λ_1 and λ_2 of a 2×2 matrix $\mathbf{A}$ have the following properties:

- Their product is equal to the determinant of $\mathbf{A}$.
- Their sum is equal to the trace of $\mathbf{A}$.

In the case of the Hessian matrix, we have

$$\begin{aligned} \lambda_1\lambda_2 &= \det \mathbf{H}, \\ \lambda_1 + \lambda_2 &= \operatorname{tr} \mathbf{H}. \end{aligned}$$

From the first of these equations we see that the condition $\det \mathbf{H} < 0$ corresponds to eigenvalues of opposite signs, and therefore to a saddle point. The condition $\det \mathbf{H} > 0$ corresponds to eigenvalues of the same sign, and therefore to an extremum – a local minimum if both eigenvalues are positive, and a local maximum if they are both negative.

In order to distinguish between these two types of extremum, we can consider $\operatorname{tr} \mathbf{H}$, which is positive for a local minimum and negative for a local maximum. We can find the sign of $\operatorname{tr} \mathbf{H}$ from its definition

$$\operatorname{tr} \mathbf{H} = f_{xx}(a,b) + f_{yy}(a,b).$$

However, there is an even simpler test. Because

$$\det \mathbf{H} = f_{xx}(a,b)\, f_{yy}(a,b) - f_{xy}^2(a,b),$$

we see that $f_{xx}(a,b)$ and $f_{yy}(a,b)$ must have the same sign if $\det \mathbf{H} > 0$. It follows that a local minimum is characterised by $\det \mathbf{H} > 0$ and $f_{xx}(a,b) > 0$, and a local maximum is characterised by $\det \mathbf{H} > 0$ and $f_{xx}(a,b) < 0$. The following box summarises the situation.

Determinant test for functions of two variables

Suppose that $f(x,y)$ is a smooth function, with a stationary point at (a,b) and a corresponding Hessian matrix $\mathbf{H}$. Then the stationary point is:

- a local minimum if $\det \mathbf{H} > 0$ and $f_{xx}(a,b) > 0$
- a local maximum if $\det \mathbf{H} > 0$ and $f_{xx}(a,b) < 0$
- a saddle point if $\det \mathbf{H} < 0$.

The test is inconclusive if $\det \mathbf{H} = 0$.

We could equally well use $f_{yy}(a,b)$ instead of $f_{xx}(a,b)$ in this test.

Exercise 27

Check that the determinant test reproduces the results derived in Example 11 and Exercise 26.

The determinant test saves a small amount of time because it avoids the need to find the eigenvalues of the Hessian matrix, but it is really an aside to our main discussion. This is because it is restricted to functions of two variables. By contrast, the eigenvalue test can be extended to functions with any number of variables. We will briefly describe how this extension works.

The definitions of stationary point, extremum, local minimum, local maximum and saddle point can all be extended in a natural way. For example, any stationary point is identified by the fact that all of its first-order partial derivatives are equal to zero. So for a function $f(x,y,z)$ of three variables, (a,b,c) is a *stationary point* if and only if

$$f_x(a,b,c) = f_y(a,b,c) = f_z(a,b,c) = 0.$$

This point is a local minimum if $f(x,y,z)$ is *greater* than $f(a,b,c)$ at all points $(x,y,z) \neq (a,b,c)$ in the immediate vicinity of (a,b,c), and so on.

The arguments leading to the eigenvalue test are also similar to those given earlier. The only difference is that the matrices $\mathbf{G}$, $\mathbf{H}$ and $\mathbf{R}$ all grow in dimension as the number of variables in the function increases. For a function of n variables, the Hessian matrix is an $n \times n$ real symmetric matrix. This has n real eigenvectors $\lambda_1, \lambda_2, \ldots, \lambda_n$, corresponding to n real orthogonal eigenvectors. So equation (52) is replaced by

$$Q(x,y) = c_1^2\lambda_1 + c_2^2\lambda_2 + \cdots + c_n^2\lambda_n,$$

where $c_1, c_2, \ldots, c_n$ are all real. Just as before, this leads directly to Procedure 1, which is already phrased in such a way that it applies to any number of eigenvalues. Here is an example for a function of three variables.

Example 12

The function

$$f(x,y,z) = x^2 + y^2 + z^2 + 3xy - 2yz$$

has a stationary point at $(0,0,0)$. Use the eigenvalue test to classify it.

Solution

The first-order partial derivatives of $f(x,y,z)$ are

$$f_x = 2x + 3y, \quad f_y = 2y + 3x - 2z, \quad f_z = 2z - 2y,$$

and the second-order partial derivatives are

$$\begin{aligned} &f_{xx} = 2, \quad f_{yy} = 2, \quad f_{zz} = 2, \\ &f_{xy} = f_{yx} = 3, \quad f_{xz} = f_{zx} = 0, \quad f_{yz} = f_{zy} = -2. \end{aligned}$$

These are constants, so the Hessian matrix at $(0,0,0)$ is

$$\mathbf{H} = \begin{bmatrix} 2 & 3 & 0 \\ 3 & 2 & -2 \\ 0 & -2 & 2 \end{bmatrix}.$$

The eigenvalues of $\mathbf{H}$ satisfy the characteristic equation

$$\begin{aligned} 0 &= \begin{vmatrix} 2-\lambda & 3 & 0 \\ 3 & 2-\lambda & -2 \\ 0 & -2 & 2-\lambda \end{vmatrix} \\ &= (2-\lambda)((2-\lambda)^2 - 4)) - 3(3)(2-\lambda) \\ &= (2-\lambda)(\lambda^2 - 4\lambda - 9). \end{aligned}$$

So one of the eigenvalues is 2, and the other two eigenvalues are given by the solutions of $\lambda^2 - 4\lambda - 9 = 0$, i.e.

$$\lambda = \frac{4 \pm \sqrt{16+36}}{2} = 2 \pm \sqrt{13}.$$

So the eigenvalues are 2, $2+\sqrt{13}$ and $2-\sqrt{13}$. There are both positive and negative eigenvalues, so the stationary point is a saddle point.

Exercise 28

Find the stationary point of the function

$$f(x,y,z) = \tfrac{5}{2}(x^2+y^2) + 2xy + z^2,$$

and use the eigenvalue test to classify it.

Exercise 29

The following functions all have stationary points at $(0,0,0)$. Where possible, use the eigenvalue test to classify these stationary points.

(a) $f(x,y,z) = x^2 + 2y^2 + 3z^2$

(b) $f(x,y,z) = x^2 + 2y^2 - 3z^2$

(c) $f(x,y,z) = x^2 + 2y^2 + 3z^4$

(d) $f(x,y,z) = x^2 + 2y^2 - 3z^4$

4.4 Constrained extrema

This final subsection is optional. It is included for interest and because it may be useful if you read other texts. It will not be assessed or examined.

So far, we have considered extrema in situations where the independent variables can vary freely. In real life, constraints must often be taken into account. For example, we might ask 'what is the maximum volume of a rectangular box?'. This question is rather pointless as posed, because we can obviously make the volume as large as we choose by building a large enough box! By contrast, the question 'what is the maximum volume of a rectangular box with a total surface area of 4 square metres?' is much more interesting. In this example, the quantity that we are maximising (the volume of the box) is subject to a constraint (the fixed surface area of the box). We are to maximise the volume *while keeping the surface area fixed*. This is a new type of problem, which we now tackle.

Constrained extrema in the real world

The problem of finding extrema subject to constraints is important in economics, business administration and many other aspects of life. Very often, we need to maximise or minimise something – a company would like to maximise its profits, or a hospital would like to minimise its fatalities. But this must be achieved with known, fixed assets.

Economists often represent the desire for a given commodity by a function called the utility function, and they assume that consumers maximise this function, subject to their budget constraints. The question that we face is: given a fixed set of assets, how can we distribute them to achieve a certain goal as fully as possible?

A whole branch of physics (statistical mechanics) is based on similar ideas. In this case, the fixed asset is energy and we work out how to distribute the total energy among the various particles in a system in such a way as to maximise the probability of a particular distribution. It turns out that some distributions are overwhelmingly more likely than others, giving us the power to predict, with practical certainty, how complicated systems containing billions of billions of particles will behave. This works for gases containing 10^{24} molecules and galaxies containing 10^{11} stars, where it would be hopeless to try to predict the detailed motion of every particle.

Suppose that we want to find the maxima or minima of a function $f(x, y)$ subject to a constraint specified by the equation $g(x, y) = c$, where c is a constant. If we could solve the equation $g(x, y) = c$ to obtain y as a function of x, we could substitute this into the function f to obtain $f(x, y(x))$. This depends only on the single variable x, so we could use the rules of ordinary calculus to find its maxima and minima. But what if we cannot solve the equation $g(x, y) = c$ for y?

Problems where the constraint is specified by an inequality are also of interest, but will not be discussed here.

The key to solving this problem is provided by Figure 27, which shows contour lines for the function $f(x, y)$ (in orange) and the curve for the function $g(x, y) = c$ (in blue). In searching for a stationary point of $f(x, y)$, we are obliged to travel along the blue curve in order to satisfy the constraint. At a point like A, the blue curve crosses contour lines of $f(x, y)$, which indicates that f is changing, so A is not a stationary point. At point B, however, the blue curve is tangential to a contour line of $f(x, y)$, and this means that f is not changing as we travel along the blue curve in the vicinity of B. We can therefore say that B is a stationary point of $f(x, y)$ subject to the constraint $g(x, y) = c$.

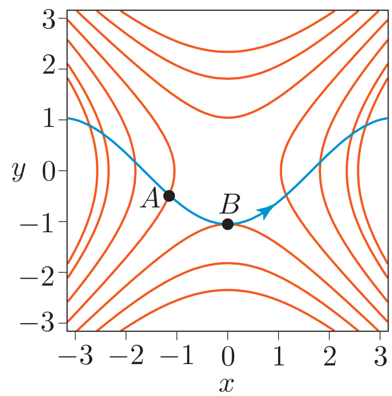


Figure 27 A situation in which we are constrained to move along the blue curve over terrain whose contour lines are shown in orange

The distinguishing feature of point B is that there is a contour line of $f(x, y)$ that is parallel to the curve $g(x, y) = c$ at point B. The corresponding gradient vectors **grad** f and **grad** g are perpendicular to these curves, so they are also aligned (parallel or antiparallel). We can therefore write

$$\mathbf{grad}\, f = \lambda\, \mathbf{grad}\, g, \tag{53}$$

where λ is a non-zero constant whose value is at present unknown. Writing down the components of equation (53), together with the original constraint, gives three equations:

We cannot say that $\lambda = 1$, because **grad** f and **grad** g may have different magnitudes.

$$\frac{\partial f}{\partial x} - \lambda \frac{\partial g}{\partial x} = 0, \quad \frac{\partial f}{\partial y} - \lambda \frac{\partial g}{\partial y} = 0, \quad g(x, y) = c. \tag{54}$$

These are 3 equations for 3 unknowns (x, y and λ), so the problem is now solved, at least in principle, by eliminating the unknown constant λ and finding values for x and y. If we let

$$L(x,y) = f(x,y) - \lambda\, g(x,y),$$

we see that equations (54) can also be written as

$$\frac{\partial L}{\partial x} = 0, \quad \frac{\partial L}{\partial y} = 0, \quad g(x,y) = c, \tag{55}$$

which leads to the following procedure.

Procedure 2 Finding stationary points with a constraint

To find the stationary points of the function $f(x,y)$ subject to the constraint $g(x,y) = c$, where c is a constant, do the following.

1. Construct the function $L(x,y) = f(x,y) - \lambda\, g(x,y)$, where λ is an unknown constant.
2. Partially differentiate $L(x,y)$ with respect to x and y, and form the equations $L_x = 0$ and $L_y = 0$.
3. Find the stationary points of $f(x,y)$ subject to the given constraint.

The following example shows how this procedure is used.

Example 13

Find the stationary points of $f(x,y) = x^2 + y^2$ subject to the constraint $xy = 4$. What are the values of f at these stationary points?

Solution

We form the function $L(x,y) = x^2 + y^2 - \lambda xy$ and calculate its first-order partial derivatives $L_x = 2x - \lambda y$ and $L_y = 2y - \lambda x$. Combining the stationary point conditions $L_x = 0$ and $L_y = 0$ with the constraint equation gives

$$2x - \lambda y = 0, \quad 2y - \lambda x = 0, \quad xy = 4.$$

Eliminating λ, we get $x^2 - y^2 = 0$. Combining this with the constraint equation then gives $x^2 - 16/x^2 = 0$, or $x^4 = 16$, which has real solutions $x = \pm 2$. Putting these values back into the constraint equation $xy = 4$, we see that there are two stationary points: $(2,2)$ and $(-2,-2)$. In each case, the corresponding value of f is $2^2 + 2^2 = 8$.

We require the solutions to be real, so imaginary solutions are rejected.

Figure 28 shows a contour map of $f(x,y) = x^2 + y^2$, with the constraint curve $xy = 4$ overlaid in blue (there is one branch for $x > 0$ and another branch for $x < 0$). You can see that the constraint curve meets the contour lines of $f(x,y)$ tangentially at the stationary points $(2,2)$ and $(-2,-2)$, and that the function f has the value 8 at these points. This is the smallest value encountered on the curve $xy = 4$, so the stationary points are local minima when the constraint is satisfied. They are not the same as the local minimum $(x,y) = (0,0)$ obtained in the absence of any constraints.

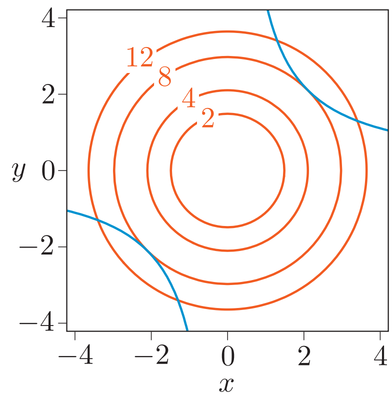


Figure 28 Contour map for $f(x,y) = x^2 + y^2$, with contour lines (orange) and constraint curve $xy = 4$ (blue)

The constant λ is called a **Lagrange multiplier**, after Joseph-Louis Lagrange (1736–1813), who devised the method that we have just described. This method works for functions of three or more variables in a very similar way, but it is not always easy to classify the stationary points. Applying the eigenvalue test to the function $L(x,y)$, for example, does not necessarily tell us the nature of the stationary points of $f(x,y)$ in the presence of a constraint. If necessary, a graph such as that in Figure 28 can be used to distinguish between the various possibilities.

Exercise 30

Find the stationary points of $f(x,y) = 5x - 3y$ subject to the constraint $x^2 - y^2 = 1$.

Learning outcomes

After studying this unit, you should be able to do the following.

- Interpret surfaces, section functions and contour maps used to represent functions of two variables.
- Calculate first- and second-order partial derivatives of a function of several variables.
- Use various versions of the chain rule.
- Calculate the first- and second-order Taylor polynomials for a function of two variables.
- Locate the stationary points of a function of two (or more) variables by solving a system of two (or more) simultaneous equations.
- Classify the stationary points of a function of two (or more) variables using the eigenvalue or determinant test.

Solutions to exercises

Solution to Exercise 1

(a) $f(2,3) = 3 \times 2^2 - 2 \times 3^2 = -6$.

(b) $f(3,-2) = 3 \times 3^2 - 2 \times (-2)^2 = 19$.

(c) $f(a,b) = 3 \times a^2 - 2 \times b^2 = 3a^2 - 2b^2$.

(d) $f(b,a) = 3 \times b^2 - 2 \times a^2 = 3b^2 - 2a^2$.

(e) $f(2a,b) = 3 \times (2a)^2 - 2 \times b^2 = 12a^2 - 2b^2$.

(f) $f(a-b,0) = 3 \times (a-b)^2 - 2 \times 0^2 = 3(a-b)^2$.

(g) $f(x,2) = 3 \times x^2 - 2 \times 2^2 = 3x^2 - 8$.

Solution to Exercise 2

We have

$$\frac{\partial g}{\partial \theta} = \cos\theta + \cos\phi \sec^2\theta \quad \text{and} \quad \frac{\partial g}{\partial \phi} = -\sin\phi \tan\theta.$$

Solution to Exercise 3

(a) Partially differentiating with respect to x, with y held constant, and using the product rule for differentiation, we get

$$f_x(x,y) = 2xe^{3x} + 3(x^2+y^2)e^{3x} = (3x^2+2x+3y^2)e^{3x}.$$

Partially differentiating with respect to y, with x held constant, gives

$$f_y(x,y) = 2ye^{3x}.$$

(b) At the point $(0,1)$, the slope of the surface in the x-direction is given by

$$f_x(0,1) = (3 \times 0^2 + 2 \times 0 + 3 \times 1^2)e^0 = 3.$$

Solution to Exercise 4

(a) Holding y and z constant,

$$\frac{\partial f}{\partial x} = 2(1+x).$$

Similarly,

$$\frac{\partial f}{\partial y} = 3(1+y)^2 \quad \text{and} \quad \frac{\partial f}{\partial z} = 4(1+z)^3.$$

(b) Holding y and t constant,

$$\frac{\partial f}{\partial x} = 2xy^3t^4 + 8xt^2 - 2y.$$

Holding x and t constant,

$$\frac{\partial f}{\partial y} = 3x^2y^2t^4 - 2x + 1.$$

Finally, holding x and y constant,

$$\frac{\partial f}{\partial t} = 4x^2y^3t^3 + 8x^2t.$$

Solution to Exercise 5

Differentiating $f(x, y) = x \sin y$ with respect to x and treating y as a constant gives

$$f_x(x, y) = \frac{\partial}{\partial x}(x \sin y) = \sin y.$$

Differentiating $f(x, y)$ with respect to y and treating x as a constant gives

$$f_y(x, y) = \frac{\partial}{\partial y}(x \sin y) = x \cos y.$$

Differentiating f_x with respect to x gives

$$f_{xx}(x, y) = \frac{\partial}{\partial x}(\sin y) = 0,$$

while differentiating f_x with respect to y gives

$$f_{yx}(x, y) = \frac{\partial}{\partial y}(\sin y) = \cos y.$$

Differentiating f_y with respect to y gives

$$f_{yy}(x, y) = \frac{\partial}{\partial y}(x \cos y) = -x \sin y,$$

while differentiating f_y with respect to x gives

$$f_{xy}(x, y) = \frac{\partial}{\partial x}(x \cos y) = \cos y.$$

Evaluating these four second-order partial derivatives at $(2, \pi)$, we get

$$\begin{aligned}
&f_{xx}(2, \pi) = 0,\\
&f_{yx}(2, \pi) = \cos \pi = -1,\\
&f_{yy}(2, \pi) = -2 \sin \pi = 0,\\
&f_{xy}(2, \pi) = \cos \pi = -1.
\end{aligned}$$

Solution to Exercise 6

The first-order partial derivatives are

$$\frac{\partial f}{\partial x} = 2e^{2x+3y} \quad \text{and} \quad \frac{\partial f}{\partial y} = 3e^{2x+3y}.$$

Partially differentiating the first of these functions with respect to y and the second with respect to x, we get

$$\begin{aligned}
f_{yx}(x, y) &= \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = 6e^{2x+3y},\\
f_{xy}(x, y) &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = 6e^{2x+3y}.
\end{aligned}$$

At the point $(x, y) = (0, 0)$, we have $f_{xy}(0, 0) = f_{yx}(0, 0) = 6$.

Solution to Exercise 7

The first-order partial derivatives are

$$\frac{\partial f}{\partial x} = -3\sin(3x-2t) \quad \text{and} \quad \frac{\partial f}{\partial t} = 2\sin(3x-2t).$$

The required second-order partial derivatives are then

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}(-3\sin(3x-2t)) = -9\cos(3x-2t),$$
$$\frac{\partial^2 f}{\partial t^2} = \frac{\partial}{\partial t}(2\sin(3x-2t)) = -4\cos(3x-2t).$$

Comparing these two expressions, we see that

$$\frac{\partial^2 f}{\partial x^2} = \frac{9}{4}\frac{\partial^2 f}{\partial t^2}, \quad \text{or equivalently,} \quad f_{xx} = \frac{9}{4} f_{tt}.$$

Solution to Exercise 8

Using the quotient rule, the first-order partial derivatives are

$$f_x(x,y) = \frac{(x+y)y - xy}{(x+y)^2} = \frac{y^2}{(x+y)^2},$$
$$f_y(x,y) = \frac{(x+y)x - xy}{(x+y)^2} = \frac{x^2}{(x+y)^2}.$$

At the initial point $(x,y) = (1,4)$, we have $f_x(1,4) = 16/25$ and $f_y(1,4) = 1/25$. We also have $\delta x = 0.01$ and $\delta y = -0.01$. The chain rule then gives

$$\delta f = f_x(1,4)\,\delta x + f_y(1,4)\,\delta y = \frac{16}{25} \times 0.01 + \frac{1}{25} \times (-0.01) = 0.006.$$

Solution to Exercise 9

Carrying out the necessary differentiations, we obtain

$$\frac{\partial z}{\partial x} = \cos x, \quad \frac{\partial z}{\partial y} = 3\sin y,$$
$$\frac{dx}{dt} = 2t, \quad \frac{dy}{dt} = 2.$$

The chain rule then gives

$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt} = 2t\cos x + 6\sin y = 2t\cos(t^2) + 6\sin(2t).$$

Solution to Exercise 10

The required derivatives are

$$\frac{\partial z}{\partial x} = y\cos x, \quad \frac{\partial z}{\partial y} = \sin x,$$
$$\frac{dx}{dt} = e^t, \quad \frac{dy}{dt} = 2t.$$

So the chain rule gives

$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt} = e^t y\cos x + 2t\sin x = t^2 e^t\cos(e^t) + 2t\sin(e^t).$$

At $t = 0$, $dz/dt = 0$.

Solution to Exercise 11

We have

$$\frac{\partial f}{\partial x} = 2x \quad \text{and} \quad \frac{\partial f}{\partial y} = 2y.$$

Also,

$$\frac{\partial x}{\partial u} = 2, \quad \frac{\partial y}{\partial u} = 3, \quad \frac{\partial x}{\partial v} = 3, \quad \frac{\partial y}{\partial v} = -2.$$

The chain rule then gives

$$\begin{aligned}\frac{\partial f}{\partial u} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial u} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial u}\\ &= 2x \times 2 + 2y \times 3 = 4(2u+3v) + 6(3u-2v) = 26u\end{aligned}$$

and

$$\begin{aligned}\frac{\partial f}{\partial v} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial v} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial v}\\ &= 2x \times 3 + 2y \times (-2) = 6(2u+3v) - 4(3u-2v) = 26v.\end{aligned}$$

At the point $(u,v) = (1,2)$, we get $f_u(1,2) = 26$ and $f_v(1,2) = 52$.

Solution to Exercise 12

We have

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial f}{\partial y} = -2y.$$

Also,

$$\frac{\partial x}{\partial r} = \cos\theta, \quad \frac{\partial y}{\partial r} = \sin\theta, \quad \frac{\partial x}{\partial \theta} = -r\sin\theta, \quad \frac{\partial y}{\partial \theta} = r\cos\theta.$$

So

$$\begin{aligned}\frac{\partial f}{\partial r} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial r}\\ &= 2x\cos\theta - 2y\sin\theta = 2r\cos^2\theta - 2r\sin^2\theta = 2r\cos(2\theta)\end{aligned}$$

and

$$\begin{aligned}\frac{\partial f}{\partial \theta} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial \theta}\\ &= 2x \times (-r\sin\theta) - 2y(r\cos\theta) = -4r^2\cos\theta\sin\theta = -2r^2\sin(2\theta).\end{aligned}$$

Solution to Exercise 13

(a) When $\widehat{\mathbf{n}}$ points in the x-direction, $\widehat{n}_x = 1$ and $\widehat{n}_y = 0$, so the slope is $f_x(x, y)$. This agrees with our previous interpretation of $\partial f/\partial x$ as the slope in the x-direction.

(b) When $\widehat{\mathbf{n}}$ points in the y-direction, $\widehat{n}_x = 0$ and $\widehat{n}_y = 1$, so the slope is $f_y(x, y)$. This agrees with our previous interpretation of $\partial f/\partial y$ as the slope in the y-direction.

Solution to Exercise 14

With $f = xy^2$, the gradient is

$$\mathbf{grad}\, f = \frac{\partial f}{\partial x}\,\mathbf{i} + \frac{\partial f}{\partial y}\,\mathbf{j} = y^2\,\mathbf{i} + 2xy\,\mathbf{j}.$$

At $(1, 2)$, this gradient has the value $2^2\,\mathbf{i} + (2 \times 1 \times 2)\,\mathbf{j} = 4\,\mathbf{i} + 4\,\mathbf{j}$.

Solution to Exercise 15

The partial derivatives are

$$\frac{\partial f}{\partial x} = 4xy^2 + 3y^3 \quad \text{and} \quad \frac{\partial f}{\partial y} = 4x^2y + 9xy^2,$$

so the gradient is

$$\mathbf{grad}\, f = (4xy^2 + 3y^3)\,\mathbf{i} + (4x^2y + 9xy^2)\,\mathbf{j}.$$

The vector $\mathbf{i} - \mathbf{j}$ is not a unit vector, but the corresponding unit vector is $\widehat{\mathbf{n}} = \frac{1}{\sqrt{2}}\,\mathbf{i} - \frac{1}{\sqrt{2}}\,\mathbf{j}$. At any point (x, y), the slope in the direction of $\widehat{\mathbf{n}}$ is

$$\begin{aligned}\widehat{\mathbf{n}} \cdot \mathbf{grad}\, f &= \frac{1}{\sqrt{2}}(4xy^2 + 3y^3) - \frac{1}{\sqrt{2}}(4x^2y + 9xy^2)\\ &= \frac{1}{\sqrt{2}}(3y^3 - 4x^2y - 5xy^2).\end{aligned}$$

Hence at $(1, 2)$, the slope in the direction of the vector $\mathbf{i} - \mathbf{j}$ is $(24 - 8 - 20)/\sqrt{2} = -2\sqrt{2} = -2.83$ (to three significant figures).

Solution to Exercise 16

Using equation (32), we see that the slope of the surface $z = f(x, y)$ is most negative when $\cos\alpha = -1$, that is, when $\alpha = \pi$. So the direction of steepest decrease at (a, b) is *opposite* to the direction of $\mathbf{grad}\, f$ at (a, b).

Solution to Exercise 17

We first calculate

$$\mathbf{grad}\, f = \frac{\partial f}{\partial x}\,\mathbf{i} + \frac{\partial f}{\partial y}\,\mathbf{j} = (4xy - 9x^2)\,\mathbf{i} + 2x^2\,\mathbf{j}.$$

At the point $(1, 2)$, this has the value

$$[\mathbf{grad}\, f]_{x=1,\,y=2} = -\mathbf{i} + 2\,\mathbf{j}.$$

This vector has magnitude $\sqrt{(-1)^2 + 2^2} = \sqrt{5}$, so the unit vector in the direction of $\mathbf{grad}\, f$ at $(1, 2)$ is $\widehat{\mathbf{n}} = (-\mathbf{i} + 2\,\mathbf{j})/\sqrt{5}$.

This is the direction of steepest *increase* of the function $f(x, y)$. The bug should move in the *opposite* direction, which is the direction of steepest *decrease* of the toxicity function. This is along the unit vector $(\mathbf{i} - 2\,\mathbf{j})/\sqrt{5}$.

Solution to Exercise 18

(a) The gradient is

$$\mathbf{grad}\, f = \frac{\partial f}{\partial x}\,\mathbf{i} + \frac{\partial f}{\partial y}\,\mathbf{j} + \frac{\partial f}{\partial z}\,\mathbf{k} = 2x\,\mathbf{i} + 2y\,\mathbf{j} + 4z\,\mathbf{k}.$$

(b) The surface of the object is a contour surface for the function $f(x, y, z)$. At each point on this surface, the gradient vector is perpendicular to the surface. At $(1, 2, 1)$ this gradient vector is

$$[\mathbf{grad}\, f]_{(1,2,1)} = 2\,\mathbf{i} + 4\,\mathbf{j} + 4\,\mathbf{k},$$

which has magnitude $\sqrt{4 + 16 + 16} = 6$. So a unit vector perpendicular to the surface at $(1, 2, 1)$ is

$$\widehat{\mathbf{n}} = \tfrac{1}{3}\,\mathbf{i} + \tfrac{2}{3}\,\mathbf{j} + \tfrac{2}{3}\,\mathbf{k}.$$

Solution to Exercise 19

(a) Example 3 found the three partial derivatives $\partial V/\partial x$, $\partial V/\partial y$ and $\partial V/\partial z$ for the function $V(x, y, z)$. Using these results, the gradient vector is

$$\mathbf{grad}\, V = -\frac{x\,\mathbf{i} + y\,\mathbf{j} + z\,\mathbf{k}}{(x^2 + y^2 + z^2)^{3/2}}.$$

(b) Because of the minus sign, $\mathbf{grad}\, V$ points in the opposite direction to the position vector $\mathbf{r} = x\,\mathbf{i} + y\,\mathbf{j} + z\,\mathbf{k}$, so we can say that at each point (x, y, z), the gradient vector $\mathbf{grad}\, V$ points towards the origin. This is the direction in which V increases most rapidly.

(c) The square of the magnitude of $\mathbf{grad}\, V$ is

$$|\mathbf{grad}\, V|^2 = \frac{x^2 + y^2 + z^2}{(x^2 + y^2 + z^2)^3} = \frac{1}{(x^2 + y^2 + z^2)^2},$$

so

$$|\mathbf{grad}\, V| = \frac{1}{x^2 + y^2 + z^2} \quad \text{for } (x, y, z) \neq (0, 0, 0).$$

Solution to Exercise 20

We have

$$f(x) = \cos x, \quad f'(x) = -\sin x, \quad f''(x) = -\cos x, \quad f'''(x) = \sin x,$$

and

$$p(x) = -1 + \tfrac{1}{2}(x - \pi)^2, \quad p'(x) = x - \pi, \quad p''(x) = 1, \quad p'''(x) = 0.$$

Hence $f(\pi) = p(\pi) = -1$, $f'(\pi) = p'(\pi) = 0$, $f''(\pi) = p''(\pi) = 1$ and $f'''(\pi) = p'''(\pi) = 0$, as required.

Solution to Exercise 21

(a) Differentiating once, and then again, gives

$$\begin{aligned} f'(t) &= \frac{1}{1+t^2} \times 2t = \frac{2t}{1+t^2}, \\ f''(t) &= \frac{(1+t^2) \times 2 - 2t \times 2t}{(1+t^2)^2} = \frac{2(1-t^2)}{(1+t^2)^2}. \end{aligned}$$

(b) At the point $t = 0$, we have $f(0) = \ln(1) = 0$, $f'(0) = 0$ and $f''(0) = 2$. So the required second-order Taylor polynomial is

$$p(t) = 0 + 0 \times t + \frac{1}{2!}\, 2 \times (t-0)^2 = t^2.$$

(c) At the point $t = 1$, we have $f(1) = \ln(2)$, $f'(1) = 1$ and $f''(1) = 0$. So the required second-order Taylor polynomial is

$$\begin{aligned} p(t) &= \ln(2) + 1 \times (t-1) + \frac{1}{2!}\, 0 \times (t-1)^2 \\ &= \ln(2) - 1 + t. \end{aligned}$$

Note that this is the *second*-order Taylor polynomial, even though it is a polynomial of order 1. This is because it takes account of the second derivative $f''(1)$, even though this turns out to be equal to zero.

Solution to Exercise 22

Setting $x = a$ and $y = b$ in equation (37), we see that $h(a,b) = p_2(a,b) = f(a,b)$, so the polynomial and the function have the same value at (a,b).

Taking first-order partial derivatives on both sides of equation (37) gives

$$\begin{aligned} h_x(x,y) &= \frac{\partial p_2}{\partial x} = f_x(a,b) + f_{xx}(a,b)(x-a) + f_{xy}(a,b)(y-b), \\ h_y(x,y) &= \frac{\partial p_2}{\partial y} = f_y(a,b) + f_{xy}(a,b)(x-a) + f_{yy}(a,b)(y-b), \end{aligned}$$

so at $x = a$ and $y = b$ we have $h_x(a,b) = f_x(a,b)$ and $h_y(a,b) = f_y(a,b)$, confirming that the first-order partial derivatives match.

Finally, differentiating again to get the second-order partial derivatives gives

$$h_{xx}(x,y) = f_{xx}(a,b), \quad h_{yy}(x,y) = f_{yy}(a,b), \quad h_{xy}(x,y) = f_{xy}(a,b).$$

In particular, we see that $h_{xx}(a,b) = f_{xx}(a,b)$, $h_{yy}(a,b) = f_{yy}(a,b)$ and $h_{xy}(a,b) = f_{xy}(a,b)$, so the second-order partial derivatives match as well.

Solution to Exercise 23

We have

$$f(x,y) = x^2 e^{3y}, \quad f_x(x,y) = 2xe^{3y}, \quad f_y(x,y) = 3x^2 e^{3y}.$$

So at $(2,0)$, we have

$$f(2,0) = 4, \quad f_x(2,0) = 4, \quad f_y(2,0) = 12.$$

Hence the first-order Taylor polynomial about $(2,0)$ is

$$\begin{aligned} p_1(x,y) &= f(2,0) + f_x(2,0)(x-2) + f_y(2,0)(y-0) \\ &= 4 + 4(x-2) + 12y \\ &= -4 + 4x + 12y. \end{aligned}$$

The second-order partial derivatives are

$$f_{xx}(x,y) = 2e^{3y}, \quad f_{xy}(x,y) = 6xe^{3y}, \quad f_{yy}(x,y) = 9x^2e^{3y}.$$

So at $(2,0)$, we have

$$f_{xx}(2,0) = 2, \quad f_{xy}(2,0) = 12, \quad f_{yy}(2,0) = 36.$$

Hence the second-order Taylor polynomial is

$$\begin{aligned} p_2(x,y) &= p_1(x,y) + \tfrac{1}{2}\big(f_{xx}(2,0)(x-2)^2 + 2f_{xy}(x-2)(y-0) \\ &\qquad\qquad\qquad + f_{yy}(2,0)(y-0)^2\big) \\ &= -4 + 4x + 12y + (x-2)^2 + 12(x-2)y + 18y^2. \end{aligned}$$

Solution to Exercise 24

Partially differentiating with respect to x and with respect to y, we obtain

$$f_x(x,y) = 6x - 4y + 4 \quad \text{and} \quad f_y(x,y) = -4x + 4y - 8.$$

Setting these first-order partial derivatives equal to zero gives

$$\begin{aligned} 6x - 4y &= -4, \\ -4x + 4y &= 8. \end{aligned}$$

These equations have the unique solution $x = 2$, $y = 4$. So $(2,4)$ is the only stationary point.

Solution to Exercise 25

We can write $f(x,y) = x^2y + xy^2 - 3xy$. Partially differentiating with respect to x and with respect to y gives

$$\begin{aligned} f_x(x,y) &= 2xy + y^2 - 3y = y(2x + y - 3), \\ f_y(x,y) &= x^2 + 2xy - 3x = x(x + 2y - 3). \end{aligned}$$

Setting these first-order partial derivatives equal to zero gives

$$\begin{aligned} y(2x + y - 3) &= 0, \\ x(x + 2y - 3) &= 0. \end{aligned}$$

Solving the first equation for y gives either $y = 0$ or $y = 3 - 2x$. For $y = 0$, the second equation becomes $x(x-3) = 0$, which is satisfied by $x = 0$ and $x = 3$. For $y = 3 - 2x$, the second equation becomes $x(3 - 3x) = 0$, which is satisfied by $x = 0$ (for which $y = 3$) and $x = 1$ (for which $y = 1$). Collecting together the complete set of solutions, the stationary points occur at $(0,0)$, $(3,0)$, $(0,3)$ and $(1,1)$.

Solution to Exercise 26

The first-order partial derivatives are

$$f_x = 4x - y - 3 \quad \text{and} \quad f_y = -x - 6y + 7.$$

Setting these equal to zero, we obtain the simultaneous equations

$$\begin{aligned} 4x - y &= 3, \\ -x - 6y &= -7, \end{aligned}$$

which have the solution $x = 1$, $y = 1$. So the only stationary point is at $(1, 1)$.

The second-order partial derivatives are $f_{xx} = 4$, $f_{yy} = -6$ and $f_{xy} = -1$. Evaluating these constant functions at $(1, 1)$ then gives $f_{xx}(1, 1) = 4$, $f_{yy}(1, 1) = -6$ and $f_{xy}(1, 1) = -1$. So the Hessian matrix at $(1, 1)$ is

$$\mathbf{H} = \begin{bmatrix} 4 & -1 \\ -1 & -6 \end{bmatrix}.$$

The eigenvalues satisfy

$$0 = \det(\mathbf{H} - \lambda\mathbf{I}) = \begin{vmatrix} 4 - \lambda & -1 \\ -1 & -6 - \lambda \end{vmatrix} = (\lambda - 4)(\lambda + 6) - 1.$$

So $\lambda^2 + 2\lambda - 25 = 0$, and the eigenvalues are

$$\lambda = \frac{-2 \pm \sqrt{104}}{2} = -1 \pm \sqrt{26}.$$

These have opposite signs, so the stationary point is a saddle point.

Solution to Exercise 27

In Example 11, the Hessian matrix at the stationary point $(0, 0)$ is

$$\mathbf{H} = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix},$$

so $\det \mathbf{H} = 4 > 0$ and $f_{xx}(0, 0) = -2 < 0$. By the determinant test, $(0, 0)$ is a local maximum.

In Exercise 26, the Hessian matrix at the stationary point $(1, 1)$ is

$$\mathbf{H} = \begin{bmatrix} 4 & -1 \\ -1 & -6 \end{bmatrix},$$

so $\det \mathbf{H} = -25 < 0$. By the determinant test, $(1, 1)$ is a saddle point.

Solution to Exercise 28

The first-order partial derivatives of $f(x, y, z)$ are

$$f_x = 5x + 2y, \quad f_y = 5y + 2x, \quad f_z = 2z.$$

The set of simultaneous equations $f_x = 0$, $f_y = 0$ and $f_z = 0$ has the unique solution $x = y = z = 0$, so the only stationary point is at $(0, 0, 0)$.

The non-zero second-order partial derivatives are

$$f_{xx} = 5, \quad f_{yy} = 5, \quad f_{zz} = 2, \quad f_{xy} = f_{yx} = 2.$$

These are constants, so the Hessian matrix at the stationary point is

$$\mathbf{H} = \begin{bmatrix} 5 & 2 & 0 \\ 2 & 5 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

The eigenvalues of this matrix are given by the characteristic equation

$$\begin{aligned} 0 &= \begin{vmatrix} 5-\lambda & 2 & 0 \\ 2 & 5-\lambda & 0 \\ 0 & 0 & 2-\lambda \end{vmatrix} \\ &= (5-\lambda)(5-\lambda)(2-\lambda) - 2(2)(2-\lambda) \\ &= (2-\lambda)(\lambda^2 - 10\lambda + 21) \\ &= (2-\lambda)(\lambda-3)(\lambda-7), \end{aligned}$$

so the eigenvalues are 2, 3 and 7. Since these are all positive, the eigenvalue test tells us that $(0,0,0)$ is a local minimum.

Solution to Exercise 29

(a) The non-zero second-order partial derivatives are $f_{xx} = 2$, $f_{yy} = 4$, $f_{zz} = 6$. These values are constants, so at the stationary point $(0,0,0)$ the Hessian matrix is

$$\mathbf{H} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 6 \end{bmatrix}.$$

This is a diagonal matrix, so its eigenvalues are 2, 4 and 6. These are all positive, so the eigenvalue test tells us that the stationary point is a local minimum.

(b) By an argument similar to that in part (a), the eigenvalues are 2, 4 and -6. These have mixed signs, so the stationary point is a saddle point.

(c) The non-zero second-order partial derivatives are $f_{xx} = 2$, $f_{yy} = 4$, $f_{zz} = 36z^2$. At the stationary point $(0,0,0)$, these have values 2, 4 and 0, giving the Hessian matrix

$$\mathbf{H} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

This is a diagonal matrix, so its eigenvalues are 2, 4 and 0. These include a zero eigenvalue, so the eigenvalue test is inconclusive. In fact, this stationary point is a local minimum, but that is not revealed by the eigenvalue test.

(d) The non-zero second-order partial derivatives are $f_{xx} = 2$, $f_{yy} = 4$, $f_{zz} = -36z^2$. At the stationary point $(0,0,0)$, these have values 2, 4 and 0, giving the same Hessian matrix as in part (c). The eigenvalue test is again inconclusive. In fact, this stationary point is a saddle point, but that is not revealed by the eigenvalue test.

Solution to Exercise 30

We form the function

$$L(x,y) = 5x - 3y - \lambda(x^2 - y^2),$$

and calculate its first-order partial derivatives $L_x = 5 - 2\lambda x$ and $L_y = -3 + 2\lambda y$. Setting these equal to zero and using the constraint equation gives

$$5 - 2\lambda x = 0, \quad -3 + 2\lambda y = 0, \quad x^2 - y^2 = 1.$$

Eliminating λ from the first two equations gives $5y - 3x = 0$, so $y = 3x/5$. Substituting this into the constraint equation, we obtain $x^2(1 - 9/25) = 1$, so $x = \pm 5/4$. We obtain the corresponding values of y from the equation $y = 3x/5$. So there are two stationary points: $(5/4, 3/4)$ and $(-5/4, -3/4)$.

Acknowledgements

Grateful acknowledgement is made to the following sources:

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